Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 11	CA/CAplus enhanced with more pre-1907 records
NEWS 7	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 8	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 9	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 10	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 11	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 12	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 13	OCT 19	E-mail format enhanced
NEWS 14	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 15	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 17	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 18	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 19	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 20	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 21	NOV 13	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 22	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 23	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 24	NOV 20	CA/CAplus patent kind codes will be updated

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that

specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:10:49 ON 30 NOV 2006

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:11:13 ON 30 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6
DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

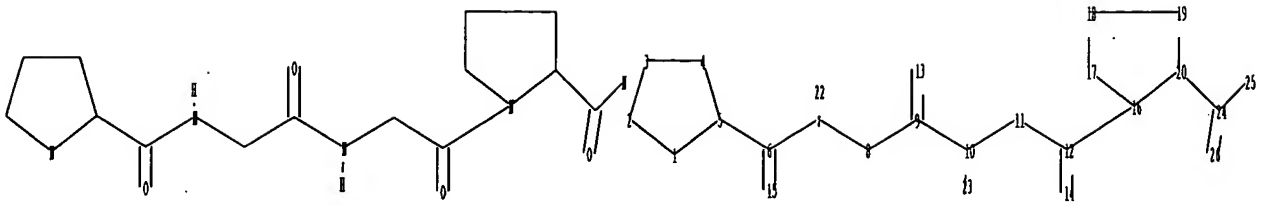
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10821663.str

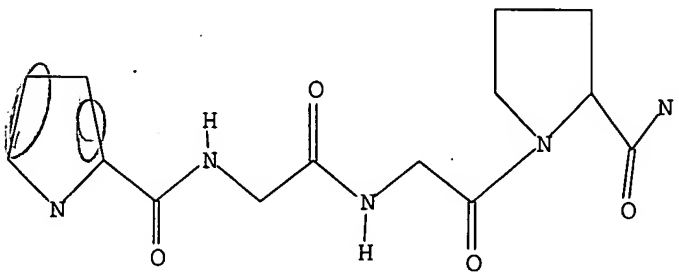


chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16
20-24 24-25 24-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20 24-25
24-26
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:11:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9936 TO ITERATE

20.1% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 192746 TO 204694
PROJECTED ANSWERS: 23297 TO 27575

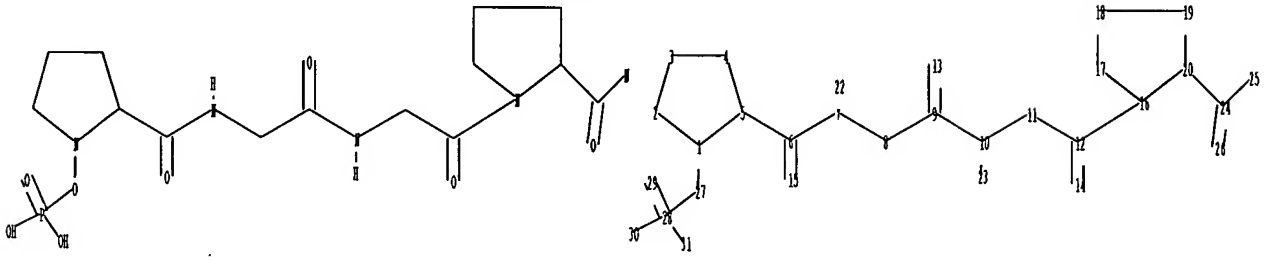
L2 50 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 14:11:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 200548 TO ITERATE

100.0% PROCESSED 200548 ITERATIONS 28521 ANSWERS
SEARCH TIME: 00.00.02

L3 28521 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10821663a.str



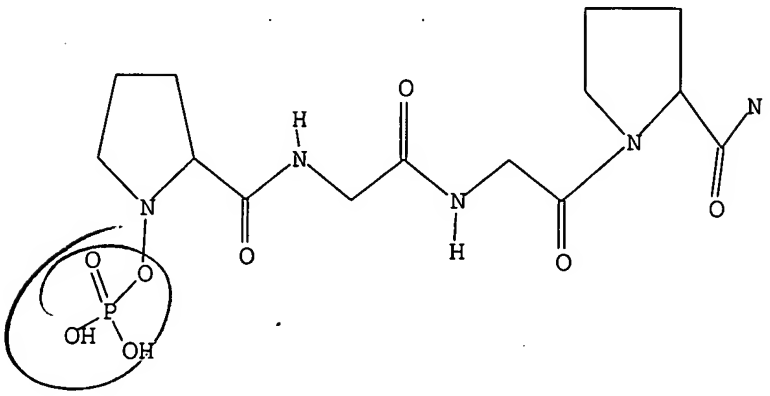
chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30 31
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
1-27 5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16
20-24 24-25 24-26 27-28 28-29 28-30 28-31
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 1-27 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20
24-25 24-26 27-28
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24
normalized bonds :
28-29 28-30 28-31
isolated ring systems :
containing 1 : 16 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS

L4 STRUCTURE UPLOADED

=> d l4
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 14:15:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

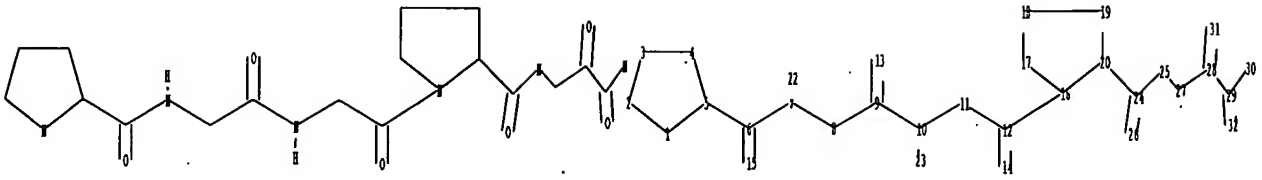
L5 0 SEA SSS SAM L4

=> s l4 sss full
FULL SEARCH INITIATED 14:15:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>
Uploading C:\Program Files\Stnexp\Queries\10821663b.str

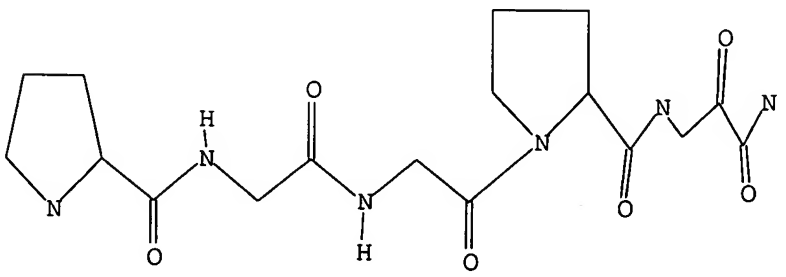


chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 32
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16
20-24 24-25 24-26 25-27 27-28 28-29 28-31 29-30 29-32
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20 24-25
24-26 25-27 28-31 29-30 29-32
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24 27-28
28-29
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS

L7 STRUCTURE UPLOADED

=> d l7
L7 HAS NO ANSWERS
L7 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l7
SAMPLE SEARCH INITIATED 14:18:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       22 TO ITERATE

100.0% PROCESSED       22 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          159 TO      721
PROJECTED ANSWERS:               0 TO        0

L8             0 SEA SSS SAM L7

=> s l7 sss full
FULL SEARCH INITIATED 14:18:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      517 TO ITERATE

100.0% PROCESSED      517 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L9             0 SEA SSS FUL L7

=>
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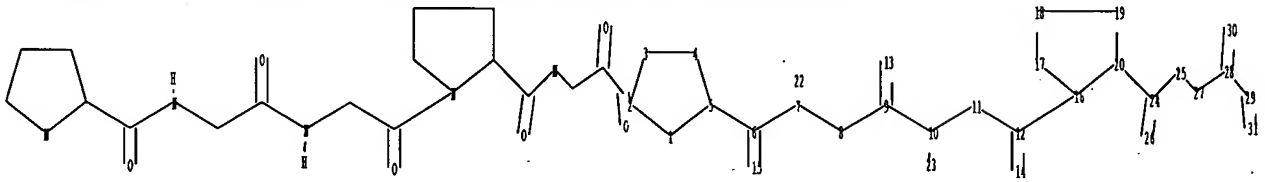
```

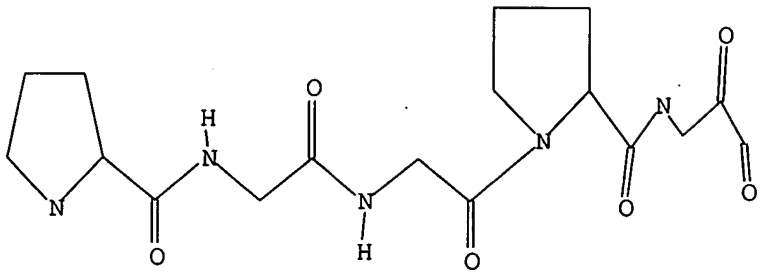


```
chain nodes :
6  7  8  9  10  11  12  13  14  15  22  23  24  25  26  27  28  29  30  31
ring nodes :
1  2  3  4  5  16  17  18  19  20
chain bonds :
5-6  6-7  6-15  7-8  7-22  8-9  9-10  9-13  10-11  10-23  11-12  12-14  12-16
20-24  24-25  24-26  25-27  27-28  28-29  28-30  29-31
ring bonds :
1-2  1-5  2-3  3-4  4-5  16-17  16-20  17-18  18-19  19-20
exact/norm bonds :
1-2  1-5  6-7  6-15  7-8  9-10  9-13  10-11  12-14  12-16  16-17  16-20  24-25
24-26  25-27  28-30  29-31
exact bonds :
2-3  3-4  4-5  5-6  7-22  8-9  10-23  11-12  17-18  18-19  19-20  20-24  27-28
28-29
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS
10:CLASS  11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom  17:Atom
18:Atom  19:Atom  20:Atom  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS
```

L10 STRUCTURE UPLOADED

=> d l10
L10 HAS NO ANSWERS
L10 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l10
SAMPLE SEARCH INITIATED 14:19:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 89 TO ITERATE

100.0% PROCESSED 89 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1214 TO 2346
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s l10 sss full
FULL SEARCH INITIATED 14:20:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1683 TO ITERATE

100.0% PROCESSED 1683 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=>
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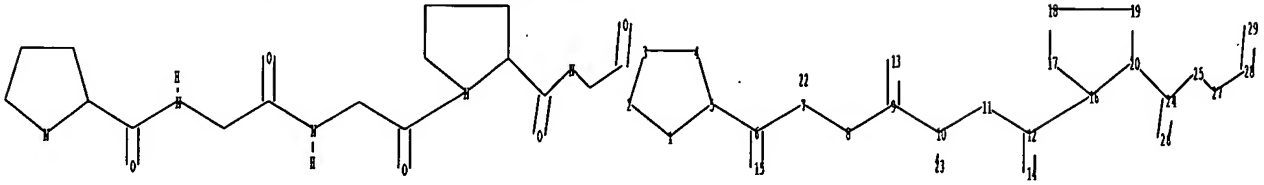
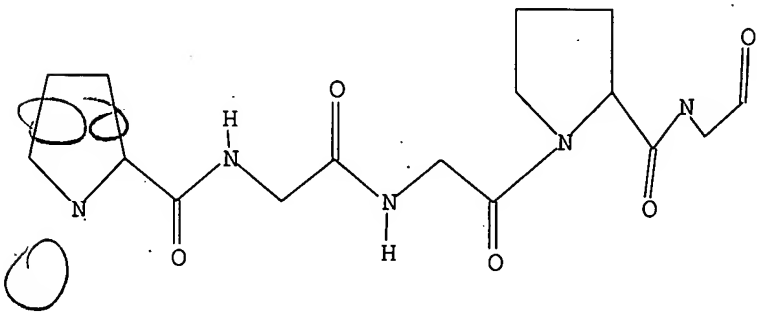


chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16
20-24 24-25 24-26 25-27 27-28 28-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20 24-25
24-26 25-27 28-29
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24 27-28
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS

L13 STRUCTURE UPLOADED

=> d l13
L13 HAS NO ANSWERS
L13 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l13
SAMPLE SEARCH INITIATED 14:21:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9936 TO ITERATE

20.1% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
PROJECTED ITERATIONS: 192746 TO 204694
PROJECTED ANSWERS: 23012 TO 27264

L14 50 SEA SSS SAM L13

=> s l13 sss full
FULL SEARCH INITIATED 14:21:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 200548 TO ITERATE

100.0% PROCESSED 200548 ITERATIONS 28214 ANSWERS
SEARCH TIME: 00.00.02

L15 28214 SEA SSS FUL L13

=>
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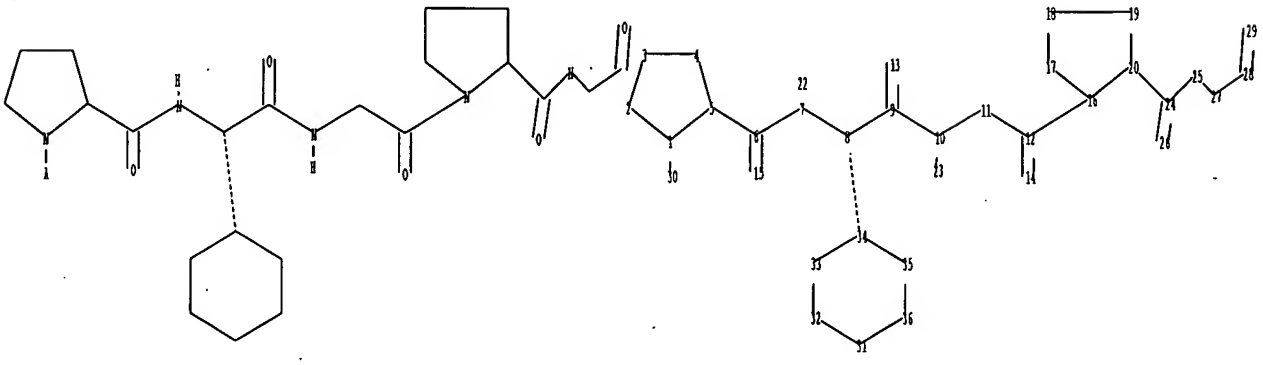
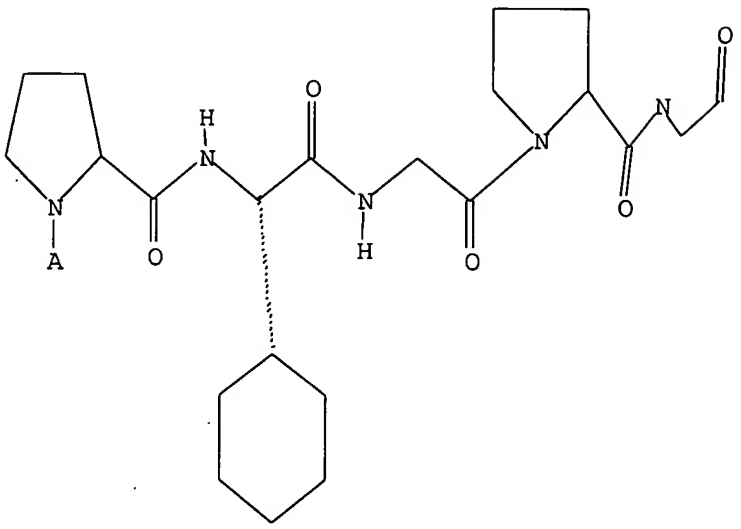


chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 16 17 18 19 20 31 32 33 34 35 36
chain bonds :
1-30 5-6 6-7 6-15 7-8 7-22 8-9 8-34 9-10 9-13 10-11 10-23 11-12 12-14
12-16 20-24 24-25 24-26 25-27 27-28 28-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20 31-32 31-36 32-33
33-34 34-35 35-36
exact/norm bonds :
1-2 1-5 1-30 6-7 6-15 7-8 8-34 9-10 9-13 10-11 12-14 12-16 16-17 16-20
24-25 24-26 25-27 28-29
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24 27-28
31-32 31-36 32-33 33-34 34-35 35-36
isolated ring systems :
containing 1 : 16 : 31 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom

L16 STRUCTURE UPLOADED

=> d l16
L16 HAS NO ANSWERS
L16 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l16
SAMPLE SEARCH INITIATED 14:24:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 137 TO ITERATE

100.0% PROCESSED 137 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2038 TO 3442
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L16

=> s l16 sss full
FULL SEARCH INITIATED 14:24:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2813 TO ITERATE

100.0% PROCESSED 2813 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L18 0 SEA SSS FUL L16

=>
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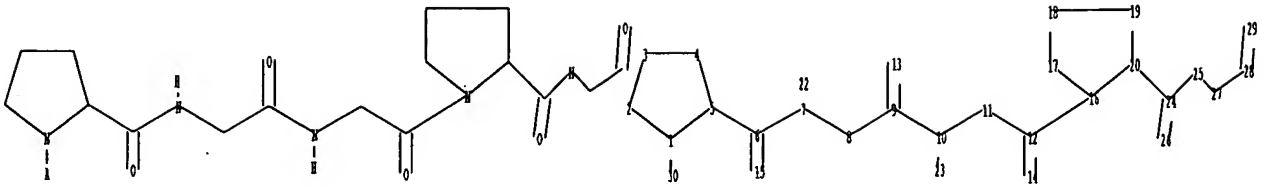
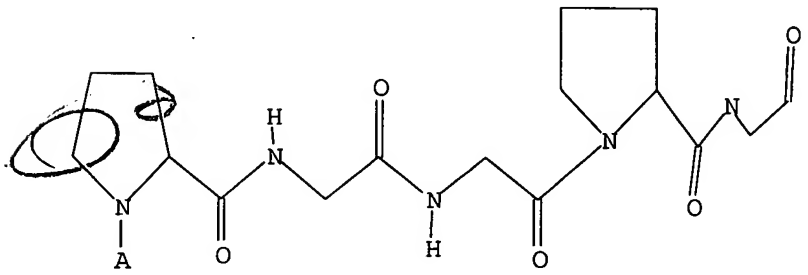


chain nodes :
6 7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30
ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
1-30 5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16
20-24 24-25 24-26 25-27 27-28 28-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 1-30 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20
24-25 24-26 25-27 28-29
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24 27-28
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS 30:CLASS

L19 STRUCTURE UPLOADED

=> d l19
L19 HAS NO ANSWERS
L19 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s l19
SAMPLE SEARCH INITIATED 14:25:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     9936 TO ITERATE

 20.1% PROCESSED     2000 ITERATIONS                                 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       192746 TO   204694
PROJECTED ANSWERS:           21300 TO    25398

L20          50 SEA SSS SAM L19

=> s l19 sss full
FULL SEARCH INITIATED 14:25:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   200548 TO ITERATE

100.0% PROCESSED   200548 ITERATIONS                          26288 ANSWERS
SEARCH TIME: 00.00.02

L21       26288 SEA SSS FUL L19

=> FIL HCAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                            1176.50    1176.71

FILE 'HCAPLUS' ENTERED AT 14:26:01 ON 30 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 30 Nov 2006  VOL 145 ISS 23
FILE LAST UPDATED: 29 Nov 2006  (20061129/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d his

     (FILE 'HOME' ENTERED AT 14:10:49 ON 30 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 14:11:13 ON 30 NOV 2006
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L21       26288 S L19 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 14:26:01 ON 30 NOV 2006

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        112763 PROTEASE
                 (PROTEASE OR PROTEASES)
        530417 INHIBITORS
         13139 PROTEASE INHIBITORS
                 (PROTEASE(W)INHIBITORS)
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=> s l23 and hepatitis
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L26          1 L23 AND HEPATITIS

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         74497 VIRUSES
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                 (VIRUS OR VIRUSES)
             2 IHHIBITOR
             1 IHHIBITORS
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             3 IHHIBITOR
               (IHHIBITOR OR IHHIBITORS)
             0 VIRUS IHHIBITOR
               (VIRUS(W)IHHIBITOR)
L27          0 L23 AND VIRUS IHHIBITOR

=> s l23 and virus
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         74497 VIRUSES
        364433 VIRUS
                 (VIRUS OR VIRUSES)
L28          9 L23 AND VIRUS

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L26  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2006:736541  HCAPLUS
DOCUMENT NUMBER:          145:180946
TITLE:                    Anti-phosphatidylserine immunoglobulin fusion products
                          for use in targeting tumor neovascularization in
                          cancer therapy
INVENTOR(S):              Thorpe, Philip E.; Luster, Troy A.; King, Steven W.
PATENT ASSIGNEE(S):       Board of Regents, The University of Texas System, USA;
                          Peregrine Pharmaceuticals, Inc.
SOURCE:                   PCT Int. Appl., 361 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
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         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006228299         A1    20061012    US 2006-339392         20060124
PRIORITY APPLN. INFO.:                       US 2005-646333P     P  20050124
AB   Fusion proteins of phosphatidylserine-binding proteins that have
     surprising combinations of properties, and a range of diagnostic and
     therapeutic uses are described. The new constructs effectively bind
     phosphatidylserine targets in disease and enhance their destruction, and
     can also specifically deliver attached imaging or therapeutic agents to
     the disease site. Also disclosed are methods of using the new construct
     compns., therapeutic conjugates and combinations thereof in tumor
     vasculature targeting, cancer diagnosis and treatment, and for treating
     viral infections and other diseases. External phosphatidylserine is shown
     to be marker of blood vessels in tumors, and absent from normal tissues,
     and so can be used as a marker for diagnosis and in the targeting of tumor
```

neovascularization in cancer therapy. Characterization of anti-phosphatidylserine antibodies and their use in targeting tumor neovascularization is reported. The antibodies are also useful in the treatment of enveloped viruses that present phosphatidylserine.

IT 716329-62-3
RL: PRP (Properties)
(unclaimed sequence; anti-phosphatidylserine Ig fusion products for use in targeting tumor neovascularization in cancer therapy)

RN 716329-62-3 HCAPLUS

CN Glycine, L-alanyl-L-seryl-L-threonyl-L-lysylglycyl-L-prolyl-L-seryl-L-valyl-L-phenylalanyl-L-prolyl-L-leucyl-L-alanyl-L-prolyl-L-seryl-L-seryl-L-lysyl-L-seryl-L-threonyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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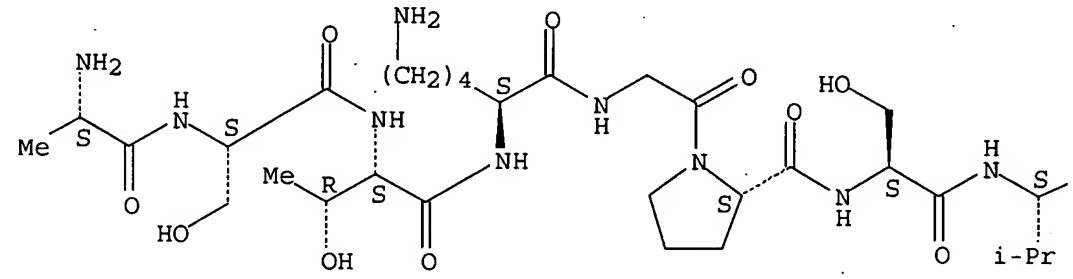

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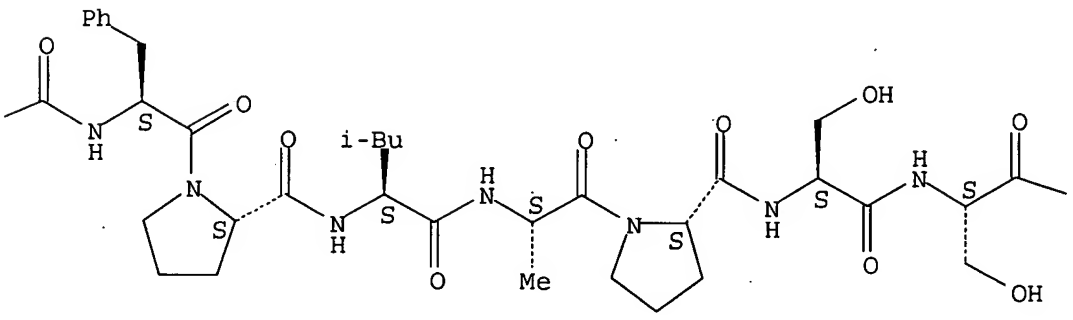

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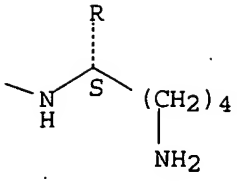

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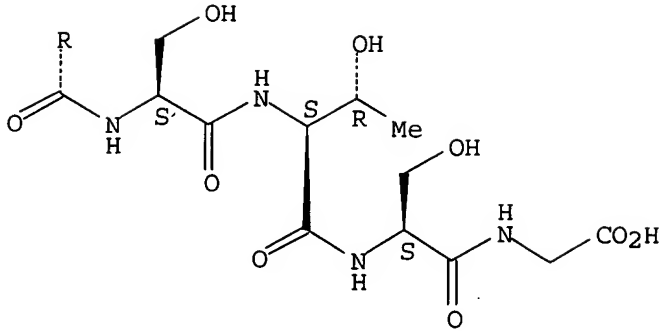

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L28 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:736541 HCAPLUS
DOCUMENT NUMBER: 145:180946
TITLE: Anti-phosphatidylserine immunoglobulin fusion products for use in targeting tumor neovascularization in cancer therapy
INVENTOR(S): Thorpe, Philip E.; Luster, Troy A.; King, Steven W.
PATENT ASSIGNEE(S): Board of Regents, The University of Texas System, USA; Peregrine Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 361 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006079120	A2	20060727	WO 2006-US2964	20060124

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,

KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

US 2006228299 A1 20061012 US 2006-339392 20060124
PRIORITY APPLN. INFO.: US 2005-646333P P 20050124

AB Fusion proteins of phosphatidylserine-binding proteins that have surprising combinations of properties, and a range of diagnostic and therapeutic uses are described. The new constructs effectively bind phosphatidylserine targets in disease and enhance their destruction, and can also specifically deliver attached imaging or therapeutic agents to the disease site. Also disclosed are methods of using the new construct compns., therapeutic conjugates and combinations thereof in tumor vasculature targeting, cancer diagnosis and treatment, and for treating viral infections and other diseases. External phosphatidylserine is shown to be marker of blood vessels in tumors, and absent from normal tissues, and so can be used as a marker for diagnosis and in the targeting of tumor neovascularization in cancer therapy. Characterization of anti-phosphatidylserine antibodies and their use in targeting tumor neovascularization is reported. The antibodies are also useful in the treatment of enveloped viruses that present phosphatidylserine.

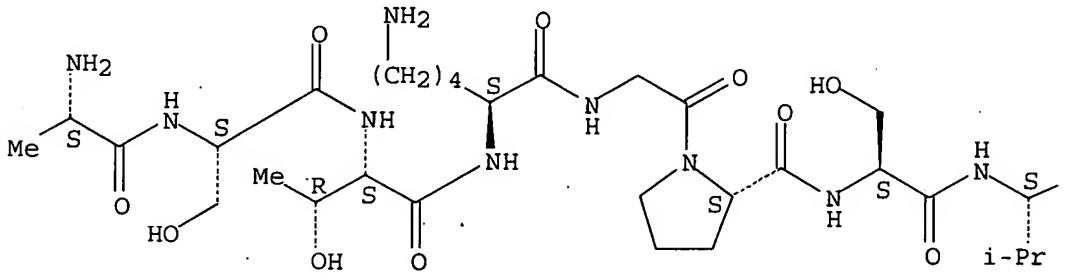
IT 716329-62-3
RL: PRP (Properties)
(unclaimed sequence; anti-phosphatidylserine Ig fusion products for use in targeting tumor neovascularization in cancer therapy)

RN 716329-62-3 HCAPLUS

CN Glycine, L-alanyl-L-seryl-L-threonyl-L-lysylglycyl-L-prolyl-L-seryl-L-valyl-L-phenylalanyl-L-prolyl-L-leucyl-L-alanyl-L-prolyl-L-seryl-L-seryl-L-lysyl-L-seryl-L-threonyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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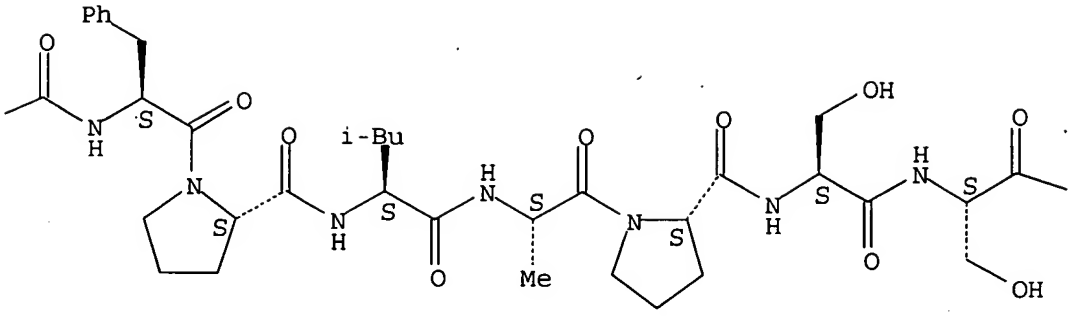

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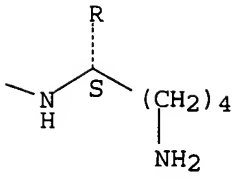

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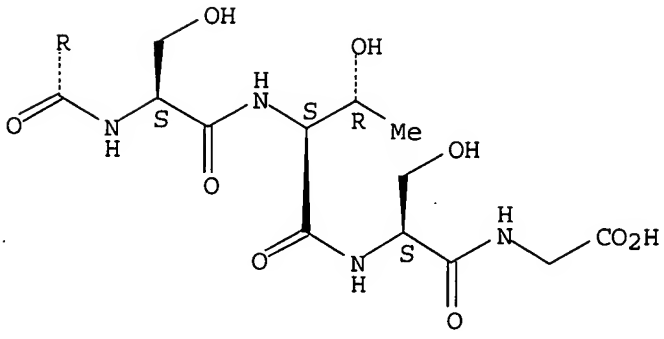


L28 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:681185 HCAPLUS
DOCUMENT NUMBER: 141:189647
TITLE: Antibodies specific to aminophospholipids, fragments and immunoconjugates for treating and diagnosing cancer and viral infections

INVENTOR(S): Thorpe, Philip E.; Soares, M. Melina; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 181 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004161429	A1	20040819	US 2003-642124		20030815
US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB Disclosed are surprising discoveries concerning the role of anionic phospholipids and aminophospholipids in tumor vasculature and in viral entry and spread, and compns. and methods for utilizing these findings in the treatment of cancer and viral infections. Also disclosed are advantageous antibody, immunoconjugate and duramycin-based compns. and combinations that bind and inhibit anionic phospholipids and aminophospholipids, for use in the safe and effective treatment of cancer, viral infections and related diseases.

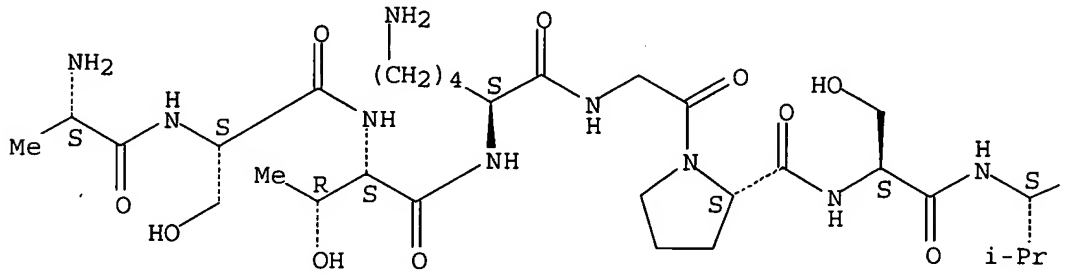
IT 716329-62-3
RL: PRP (Properties)
(unclaimed sequence; antibodies specific to aminophospholipids, fragments and immunoconjugates for treating and diagnosing cancer and viral infections)

RN 716329-62-3 HCAPLUS

CN Glycine, L-alanyl-L-seryl-L-threonyl-L-lysylglycyl-L-prolyl-L-seryl-L-valyl-L-phenylalanyl-L-prolyl-L-leucyl-L-alanyl-L-prolyl-L-seryl-L-seryl-L-lysyl-L-seryl-L-threonyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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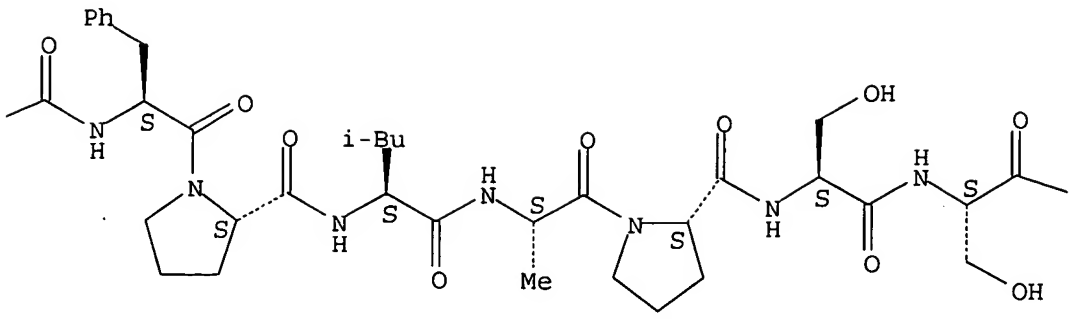

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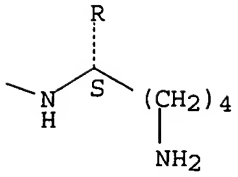

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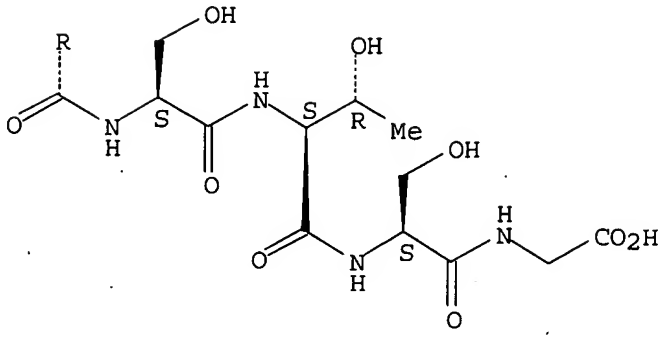

L28 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:550531 HCAPLUS
DOCUMENT NUMBER: 141:105253
TITLE: Antibodies specific to aminophospholipid and conjugates for diagnosis and treatment of cancer and viral infection

INVENTOR(S): Thorpe, Philip E.; Soares, M. Melina; Ran, Sophia
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 178 pp., Cont.-in-part of U.S. Ser. No. 621,269.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 17
PATENT INFORMATION:

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US 2004170620	A1	20040902	US 2003-621269		20030715
PRIORITY APPLN. INFO.:			US 2002-396263P	P	20020715
			US 2003-621269	A2	20030715

AB Disclosed are surprising discoveries concerning the role of anionic phospholipids and aminophospholipids in tumor vasculature and in viral entry and spread, and compns. and methods for utilizing these findings in the treatment of cancer and viral infections. Also disclosed are advantageous antibody, immunoconjugate and duramycin-based compns. and combinations that bind and inhibit anionic phospholipids and aminophospholipids, for use in the safe and effective treatment of cancer, viral infections and related diseases.

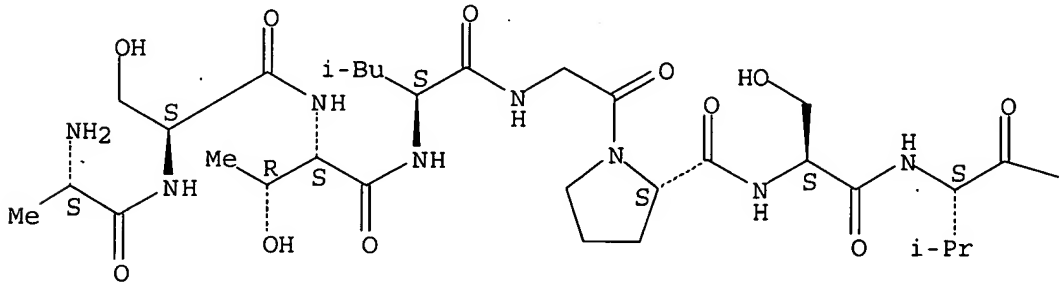
IT 650591-59-6
RL: PRP (Properties)
(unclaimed sequence; antibodies specific to aminophospholipid and conjugates for diagnosis and treatment of cancer and viral infection)

RN 650591-59-6 HCAPLUS

CN Glycine, L-alanyl-L-seryl-L-threonyl-L-leucylglycyl-L-prolyl-L-seryl-L-valyl-L-phenylalanyl-L-prolyl-L-leucyl-L-alanyl-L-prolyl-L-seryl-L-seryl-L-lysyl-L-seryl-L-threonyl-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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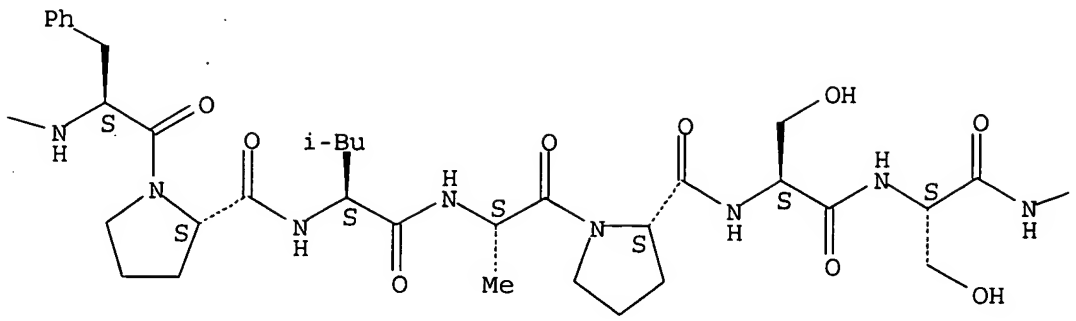

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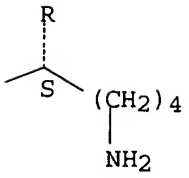

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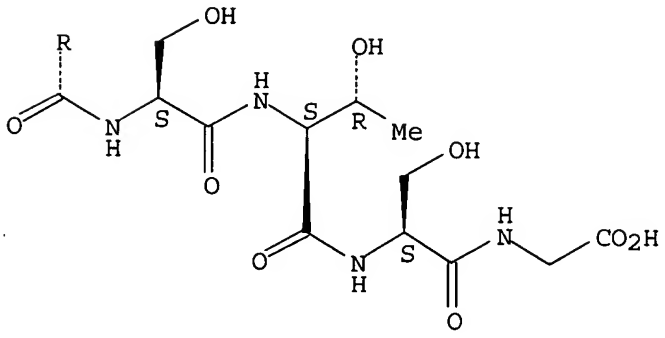

L28 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:521462 HCAPLUS
DOCUMENT NUMBER: 137:88442
TITLE: Incensole and furanogermacrens and compounds in treatment for inhibiting neoplastic lesions and microorganisms
INVENTOR(S): Shanahan-Pendergast, Elisabeth

PATENT ASSIGNEE(S): Ire.
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002053138	A2	20020711	WO 2002-IE1	20020102
WO 2002053138	A3	20020919		
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, AT, BE, CH, CY, DE, ES, FI, ML, MR, NE, SN, TD, TG				
AU 2002219472	A1	20020716	AU 2002-219472	20020102
EP 1351678	A2	20031015	EP 2002-727007	20020102
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2004092583	A1	20040513	US 2004-250535	20040102
PRIORITY APPLN. INFO.:			IE 2001-2 A	20010102
			WO 2002-IE1 W	20020102

OTHER SOURCE(S): MARPAT 137:88442

AB The invention discloses the use of incensole and/or furanogermacrens, derivs. metabolites and precursors thereof in the treatment of neoplasia, particularly resistant neoplasia and immunodysregulatory disorders. These compds. can be administered alone or in combination with conventional chemotherapeutic, antiviral, antiparasite agents, radiation and/or surgery. Incensole and furanogermacren and their mixture showed antitumor activity against various human carcinomas and melanomas and antimicrobial activity against Staphylococcus aureus and Enterococcus faecalis.

IT 154277-21-1, Cypemycin
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical formulation further including; incensole and furanogermacrens and compds. as antitumor and antimicrobial agents)

RN 154277-21-1 HCAPLUS
CN Cypemycin (9CI) (CA INDEX NAME)

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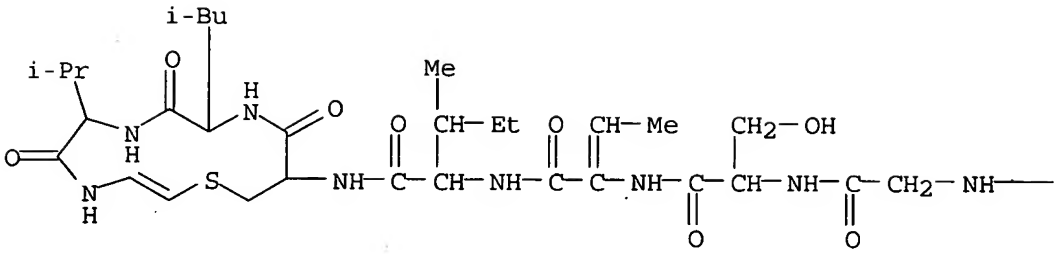

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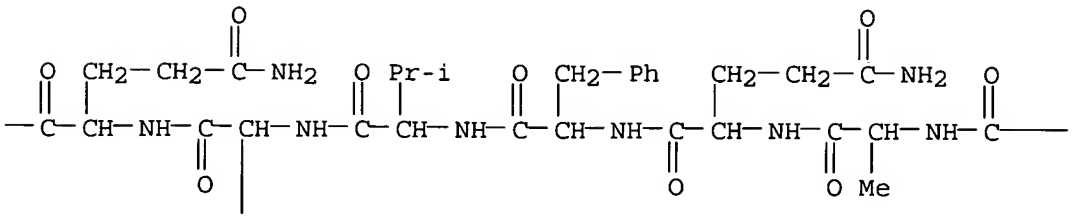

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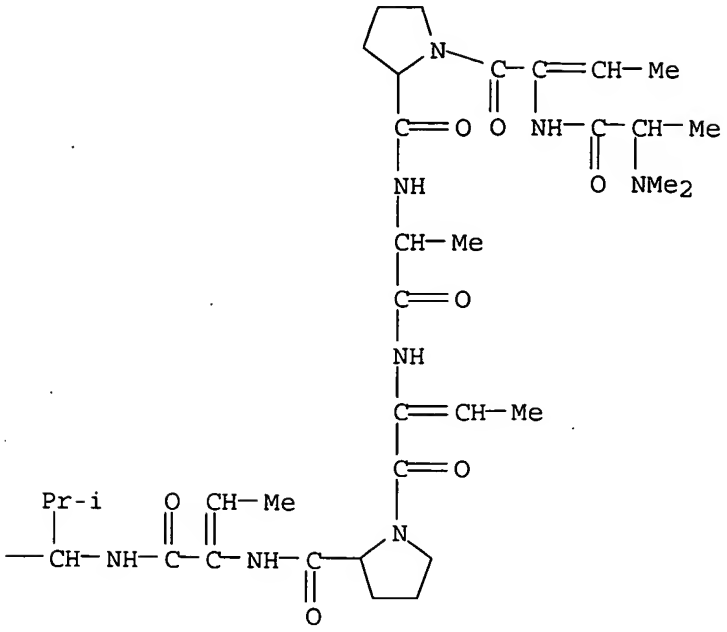

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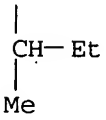


L28 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:185159 HCAPLUS
DOCUMENT NUMBER: 136:244041
TITLE: A method for identifying peptide sequences having a specific functionality
INVENTOR(S): Schneider, Gisbert; Eichler-Mertens, Mathias; Wrede, Paul
PATENT ASSIGNEE(S): Callistogen A.-G., Germany
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020564	A2	20020314	WO 2001-EP10195	20010905
WO 2002020564	A3	20031002		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,

PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

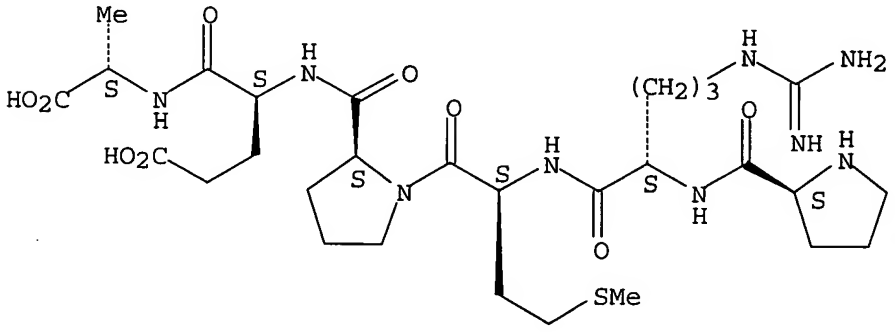
AU 2001093794 A5 20020322 AU 2001-93794 20010905
PRIORITY APPLN. INFO.: US 2000-655056 A 20000905
WO 2001-EP10195 W 20010905

AB The present invention relates to a method for creating a sequence-function relationship, a method for identifying or generating peptide sequences having a specific functionality, using the created sequence-function relationship and a method for generating a focussed synthetic peptide library. The PepHarvester algorithm was applied to the HSP70 binding peptide LHIYTT. By using a diversity index of 0.1, 40 variants were created.

IT 403667-35-6 403667-55-0
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(amino acid sequence, as calculated HSP70-binding peptide in protein p53; method for identifying peptide sequences having a specific functionality)

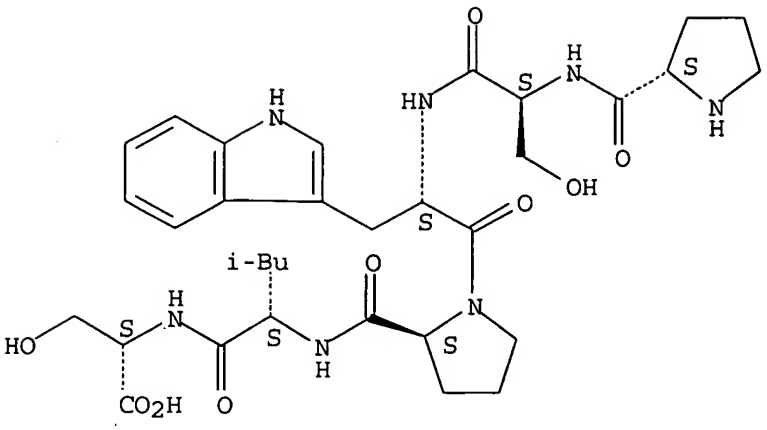
RN 403667-35-6 HCAPLUS
CN L-Alanine, L-prolyl-L-arginyl-L-methionyl-L-prolyl-L-α-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 403667-55-0 HCAPLUS
CN L-Serine, L-prolyl-L-seryl-L-tryptophyl-L-prolyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:661566 HCAPLUS
DOCUMENT NUMBER: 135:223436
TITLE: Recombinant adenyl cyclase and use thereof for screening for proteolytic activity and protease inhibitors
INVENTOR(S): Karimova, Gouzel; Ladant, Daniel; Ullmann, Agnes; Dautin, Nathalie
PATENT ASSIGNEE(S): Institut Pasteur, Fr.; Centre National de la Recherche Scientifique (CNRS)
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064854	A1	20010907	WO 2001-FR593	20010228
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2805544	A1	20010831	FR 2000-2448	20000228
FR 2805544	B1	20040716		
CA 2401315	AA	20010907	CA 2001-2401315	20010228
BR 2001008767	A	20021203	BR 2001-8767	20010228
EP 1265993	A1	20021218	EP 2001-909931	20010228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003525606	T2	20030902	JP 2001-564337	20010228
US 2003175735	A1	20030918	US 2002-204987	20021218
PRIORITY APPLN. INFO.:			FR 2000-2448 A	20000228
			WO 2001-FR593 W	20010228

AB The invention concerns a recombinant adenyl cyclase, comprising at least one protease cleavage site, said site being inserted into the catalytic domain of the adenyl cyclase while preserving its enzymic activity. The invention also concerns methods for screening mols. with proteolytic activity using said recombinant adenyl cyclase. Thus, cya- E. coli were transformed with plasmids encoding Bordetella pertussis adenyl cyclase catalytic domain. An HIV proteinase cleavage site was inserted between residues 224 and 225 of the catalytic domain. In the absence of HIV proteinase these recombinant bacteria formed red colonies on McConkey maltose plates, while in the presence of HIV proteinase the colonies were white. An assay sensitive enough for saquinavir or indinavir-resistant HIV proteinase was provided by cya- E. coli producing adenyl cyclase catalytic domain containing the HIV proteinase flanked by HIV proteinase cleavage sites.

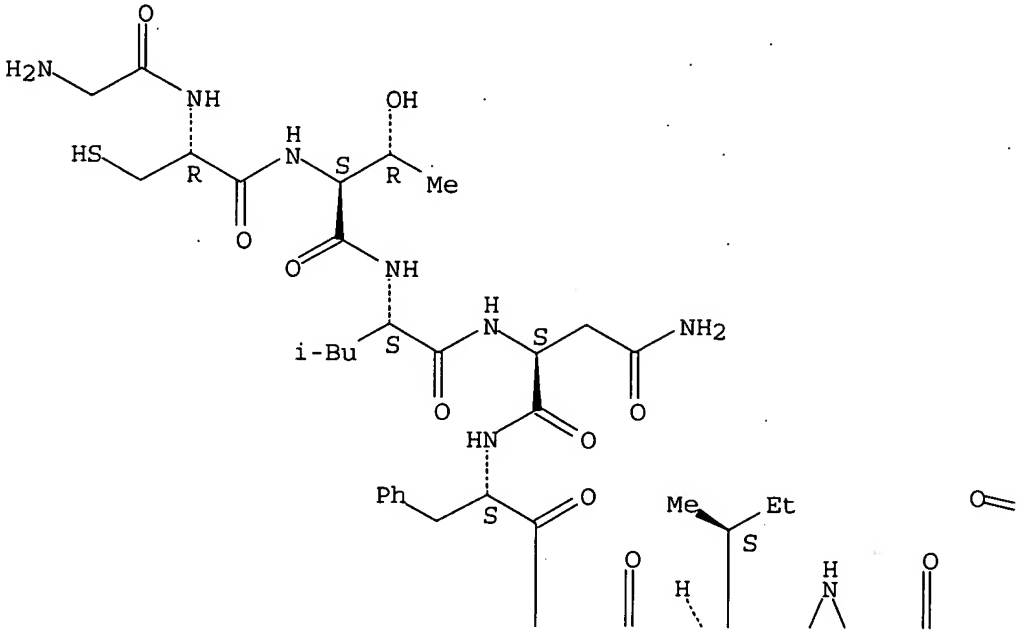
IT 358628-09-8
RL: BOC (Biological occurrence); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence); PROC (Process)
(HIV proteinase cleavage site; recombinant adenyl cyclase and use thereof for screening for proteolytic activity and protease inhibitors)

RN 358628-09-8 HCAPLUS

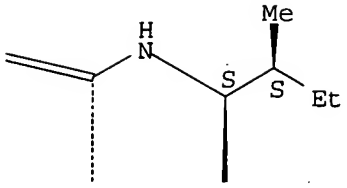
CN L-Glutamic acid, glycyl-L-cysteinyl-L-threonyl-L-leucyl-L-asparaginyl-L-phenylalanyl-L-prolyl-L-isoleucyl-L-seryl-L-prolyl-L-isoleucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

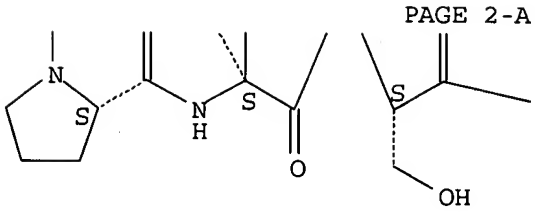
PAGE 1-A



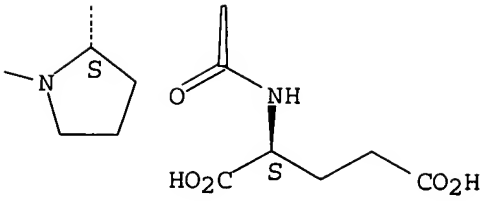
PAGE 1-B



PAGE 2-A



PAGE 2-B



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

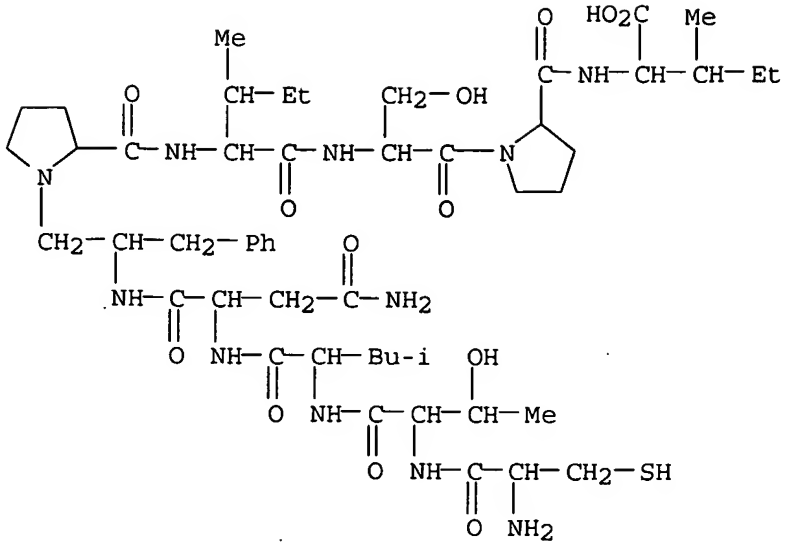
L28 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:409303 HCAPLUS
DOCUMENT NUMBER: 115:9303
TITLE: Development of methodology for the synthesis of stereochemically pure Pheψ[CH2N]Pro linkages in HIV protease inhibitors

AUTHOR(S): Cushman, Mark; Oh, Young Im; Copeland, Terry D.; Oroszlan, Stephen; Snyder, Stuart W.
CORPORATE SOURCE: Sch. Pharm. Pharmacal Sci., Purdue Univ., West Lafayette, IN, 47907, USA
SOURCE: Journal of Organic Chemistry (1991), 56(13), 4161-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:9303

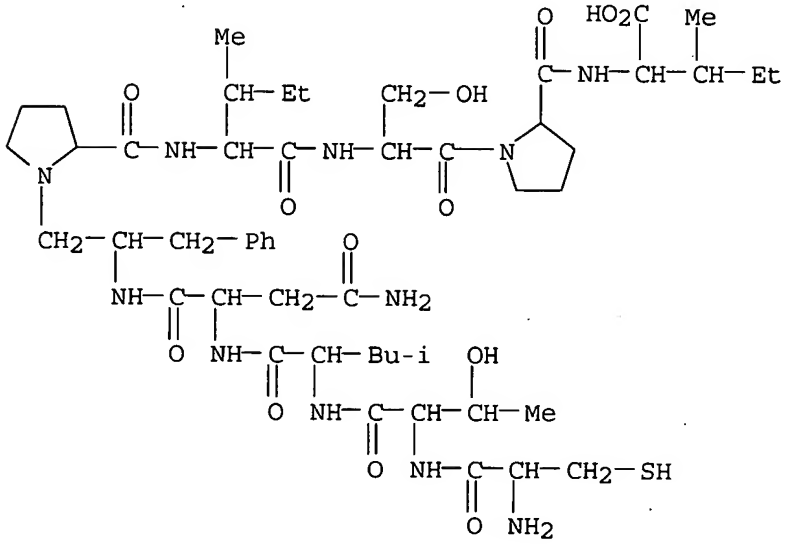
AB One of the strategies currently being pursued for the design of potential HIV protease inhibitors involves the replacement of the cleaved amide bond in a min. peptide substrate with an aminomethylene unit. A commonly used method for the synthesis of these compds. involves a reductive alkylation of an amine with an aldehyde in the presence of sodium cyanoborohydride under acidic conditions. Accordingly, Boc-phenylalaninal (Boc = Me3CO2C) was treated with H-Pro-Ile-Ser(CH2Ph)-O-resin in the presence of acetic acid and sodium cyanoborohydride. The resulting product was found to consist of a mixture of diastereomers, which may result from the fact that the proline residue, which contains a secondary amine, reacts with the aldehyde to form an enamine with loss of chirality at the modified Phe residue. Subsequent reduction of the iminium ion would then result in production of the observed two diastereomers. In order to circumvent this problem, the central amide bond of Boc-Phe-Pro-OCH2Ph was reduced selectively with B2H6 to give Boc-Pheψ[CH2N]Pro-OR (I, R = CH2Ph), which underwent hydrogenolysis to give I (R = H). The latter was coupled with H-Ile-Ser(CH2Ph)-O-resin to give Boc-Pheψ[CH2N]Pro-Ile-Ser(CH2Ph)-O-resin (II). Subsequent addition of amino acid residues to II and cleavage from the resin gave a series of stereochem. defined potential HIV protease inhibitors as single diastereomers. The most potent of these substances was H-Thr-Leu-Asn-Pheψ[CH2N]-Pro-Ile-Ser (III) which displayed an IC50 of 1.1 μg/mL (1.4 μM) when tested for inhibition of HIV-1 protease. However, the epimer of III having the opposite configuration at the reduced Phe residue was inactive. A min. length of seven amino acid residues appears to be necessary for effective recognition of the inhibitor by the enzyme. Further increase in chain length did not result in greater inhibitory potency.

IT 133673-10-6P 133773-54-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition by, of HIV protease)

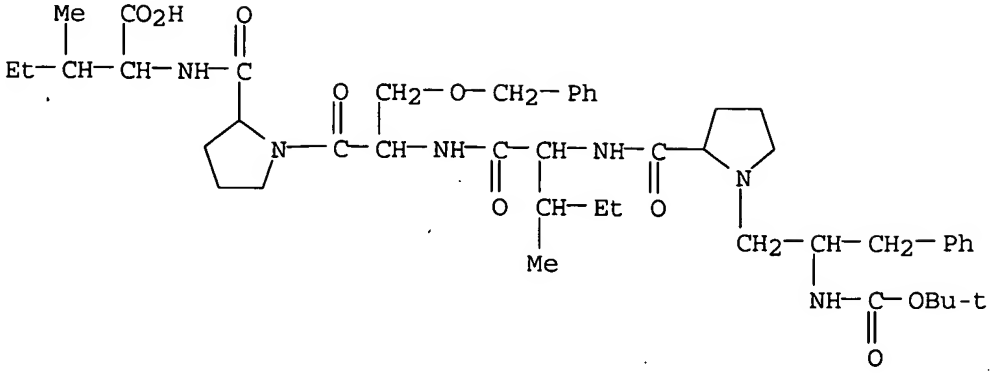
RN 133673-10-6 HCAPLUS
CN L-Isoleucine, N-[1-[N-[N-[1-[2-[[N2-[N-(N-L-cysteinyl-L-threonyl)-L-leucyl]-L-asparaginyl]amino]-3-phenylpropyl]-L-prolyl]-L-isoleucyl]-L-seryl]-L-prolyl]-, (S)- (9CI) (CA INDEX NAME)



RN 133773-54-3 HCAPLUS
CN L-Isoleucine, N-[1-[N-[N-[1-[2-[[N2-[N-(N-L-cysteinyl-L-threonyl)-L-leucyl]-L-asparaginyl]amino]-3-phenylpropyl]-L-prolyl]-L-isoleucyl]-L-seryl]-L-prolyl]-, (R)- (9CI) (CA INDEX NAME)



IT 133673-20-8DP, resin-bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in solid-phase synthesis of aminomethylene pseudopeptide)
RN 133673-20-8 HCAPLUS
CN L-Isoleucine, N-[1-[N-[N-[1-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-phenylpropyl]-L-prolyl]-L-isoleucyl]-O-(phenylmethyl)-L-seryl]-L-prolyl]-, (S)- (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:402499 HCAPLUS
DOCUMENT NUMBER: 115:2499
TITLE: Recombinant hybrid protease inhibitors and their use
INVENTOR(S): Ringe, Dagmar
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9100912	A1	19910124	WO 1990-US3769	19900703
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				

PRIORITY APPLN. INFO.: US 1989-376876 A 19890707

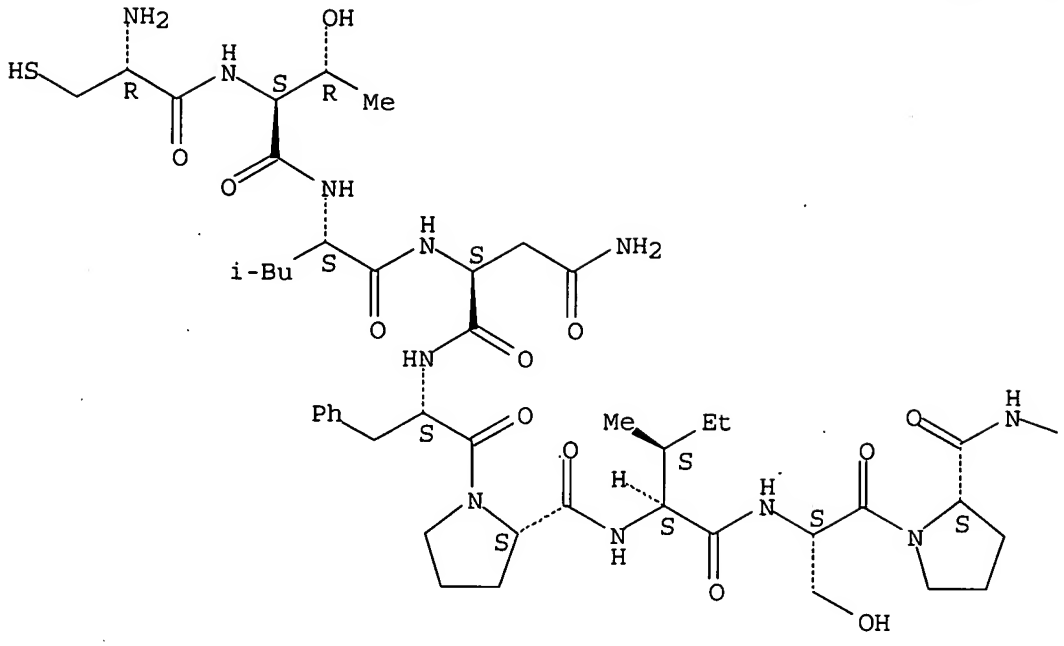
AB A highly specific hybrid protease inhibitor comprises a nonimmunogenic carrier polypeptide having an internal portion replaced/expanded with a synthetic peptide that specifically binds and inhibits a protease. The hybrid protease inhibitor also exhibits longer in vivo half-life than the synthetic peptide per se, which is desirable for clin. applications. Preparation of hybrid protease inhibitors that are inhibitory to elastase, chymotrypsin, trypsin, HIV protease, thrombin, and renin, resp., using interleukin-1 β as a nonimmunogenic carrier polypeptide are demonstrated.

IT 118071-38-8
RL: PRP (Properties)
(HIV protease recognition and inhibition site, synthetic, hybrid inhibitor containing interleukin 1-β and)

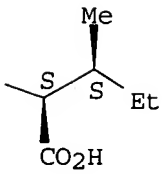
RN 118071-38-8 HCAPLUS
CN L-Isoleucine, L-cysteinyl-L-threonyl-L-leucyl-L-asparaginyl-L-phenylalanyl-L-prolyl-L-isoleucyl-L-seryl-L-prolyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L28 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:553045 HCAPLUS
DOCUMENT NUMBER: 113:153045
TITLE: Preparation of retroviral protease-inhibiting peptides and pharmaceutical compositions containing them
INVENTOR(S): Dreyer, Geoffrey Bainbridge; Huffman, William Francis; Meek, Thomas Dowing; Metcalf, Brian Walter; Moore, Michael Lee

PATENT ASSIGNEE(S): SmithKline Beckman Corp., USA
SOURCE: Eur. Pat. Appl., 118 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 352000	A2	19900124	EP 1989-306995		19890710
EP 352000	A3	19910717			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
ZA 8905174	A	19900328	ZA 1989-5174		19890707
CN 1039596	A	19900214	CN 1989-104699		19890708
PRIORITY APPLN. INFO.:			US 1988-216178	A	19880708
			US 1989-321937	A	19890310

OTHER SOURCE(S): MARPAT 113:153045

AB A-B-(Q)a-(C)b-(D)c-M-(W)d-(X)e-Y-Z [I; A = H, protecting group, (protected) amino, alkanamido, etc.; B = D- or L-amino acid residue, e.g., β-Ala, bond; C, D = Glx, Asx, Ala, β-Ala, Arg, Gly, Ile, Leu, Lys, Ser, Thr, Val, Met, His; Asx = Asp, Asn; Glx = Glu, Gln; Q = D- or L-amino acid residue, e.g.; Ser, Thr, Asp, His, Cys, Arg, Ala; W = Pro, dehydro-Pro; X = Ala, Gly, Ile, Leu, Val, Met, Lys, Glx, Asx; Y = D- or L-amino acid residue(s), bond; Z = CO2H, alkoxycarbonyl, (substituted) amino, etc.; a-e = 0, 1, however, c and e may not simultaneously be 0; M = Cha, (substituted) Phe, alkylamino] and their pharmaceutically acceptable salts were prepared Many I, e.g., Ac-Ser-Gln-Ser-Tyr-Pro-Val-Val-NH2, were prepared by solid-phase or solution synthesis. 2-(Acetylserylglutaminylasparaginyl)amino-3-phenylpropylprolylvalylvalinamide (preparation given) showed an inhibition constant Ki of 14 μM in vitro against rHIV protease. Many pharmaceutical dosage forms containing 1 were formulated.

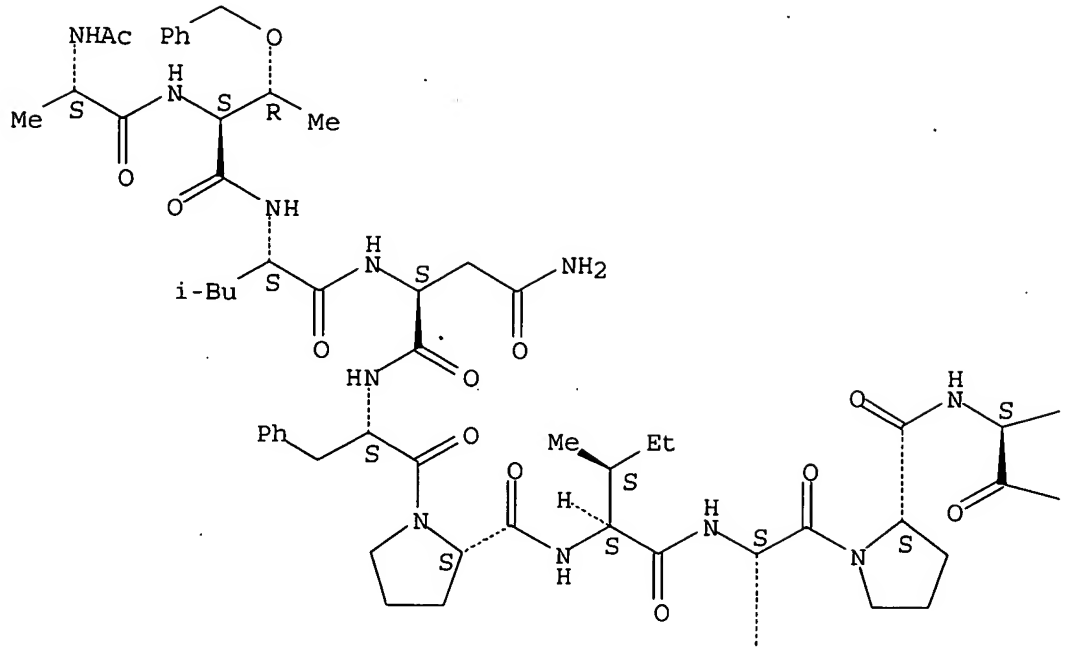
IT 128212-20-4DP, benzhydrylamine resin bound
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for retroviral protease inhibitor)

RN 128212-20-4 HCAPLUS

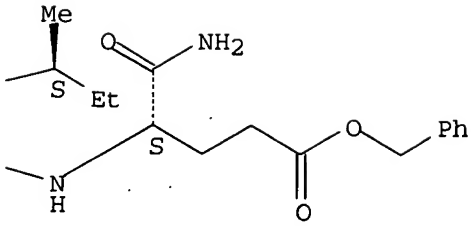
CN L-α-Glutamine, N2-[N-[1-[N-[N-[1-[N-[N2-[N-[N-(N-acetyl-L-alanyl)-O-(phenylmethyl)-L-threonyl]-L-leucyl]-L-asparaginyl]-L-phenylalanyl]-L-prolyl]-L-isoleucyl]-O-(phenylmethyl)-L-seryl]-L-prolyl]-L-isoleucyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

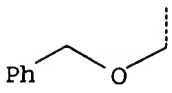
PAGE 1-A



PAGE 1-B



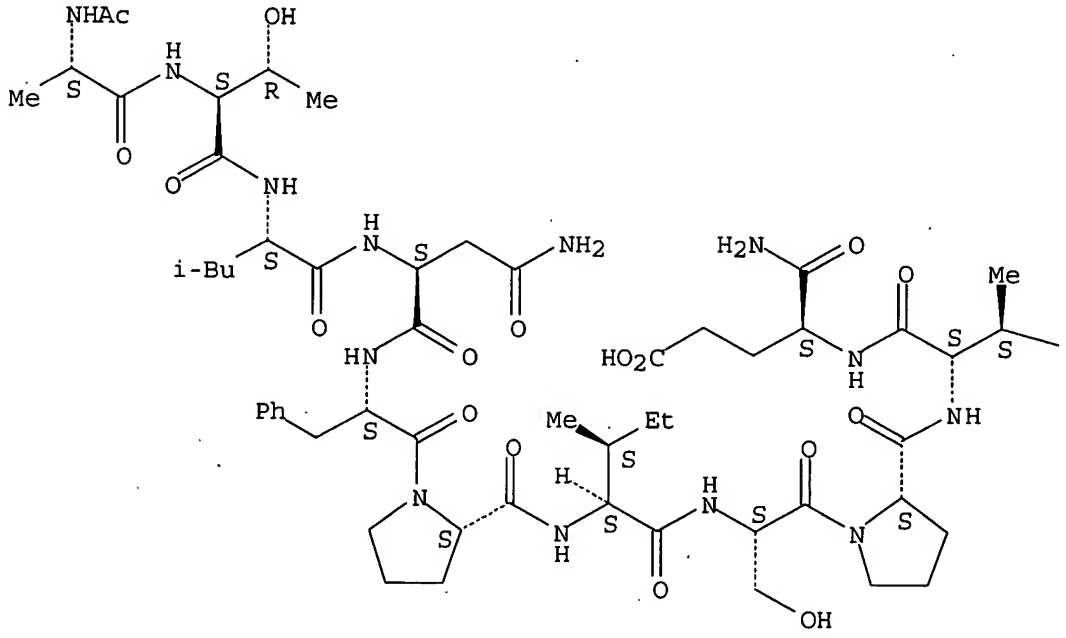
PAGE 2-A



IT 128210-64-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as viral protease inhibitor)
RN 128210-64-0 HCAPLUS
CN L-α-Glutamine, N2-[N-[1-[N-[N-[1-[N-[N2-[N-[N-(N-acetyl-L-alanyl)-L-threonyl]-L-leucyl]-L-asparaginyl]-L-phenylalanyl]-L-prolyl]-L-isoleucyl]-L-seryl]-L-prolyl]-L-isoleucyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

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FULL ESTIMATED COST	76.40	1253.11

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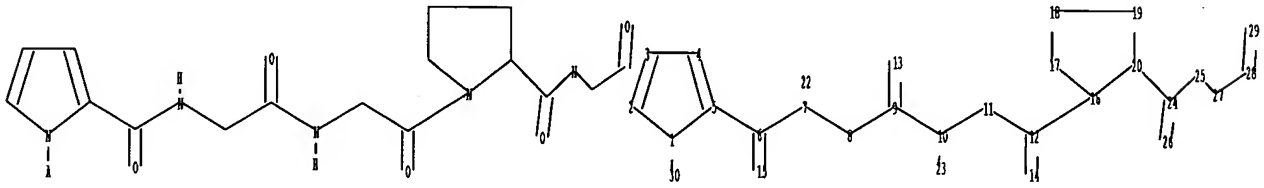

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ring nodes :
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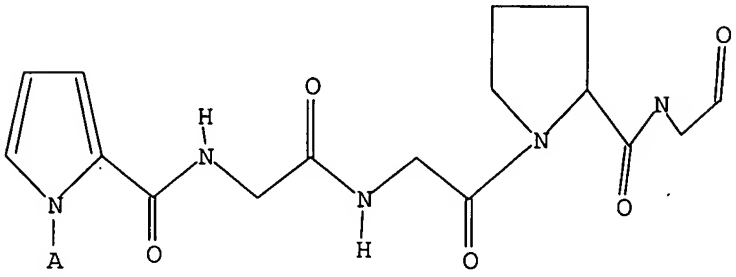
1-30 5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16 20-24 24-25 24-26 25-27 27-28 28-29
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 1-30 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20 24-25 24-26 25-27 28-29
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24 27-28
isolated ring systems :

containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS 30:CLASS

L29 STRUCTURE UPLOADED

=> d l29
L29 HAS NO ANSWERS
L29 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l29
SAMPLE SEARCH INITIATED 14:32:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 190 TO ITERATE

100.0% PROCESSED 190 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2973 TO 4627
PROJECTED ANSWERS: 0 TO 0

L30 0 SEA SSS SAM L29

=> s l29 sss full
FULL SEARCH INITIATED 14:32:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4166 TO ITERATE

100.0% PROCESSED 4166 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L31 1 SEA SSS FUL L29

=> FIL HCAPLUS
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST	166.94	1420.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.50

FILE 'HCAPLUS' ENTERED AT 14:32:38 ON 30 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23
FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l31
L32 3 L31

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.06	1425.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-7.50

FILE 'REGISTRY' ENTERED AT 14:33:42 ON 30 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6
DICTIONARY FILE UPDATES: 29 NOV 2006 HIGHEST RN 914337-13-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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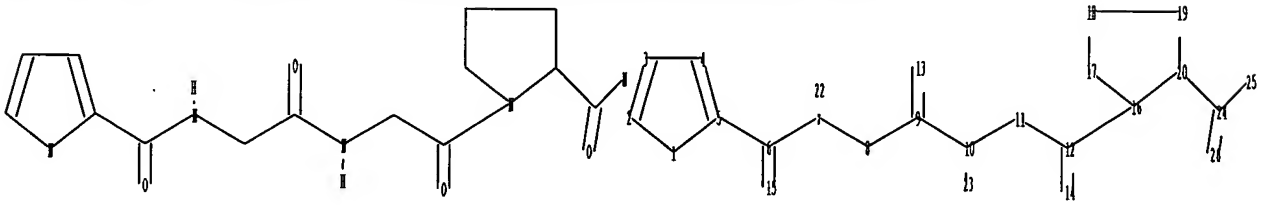
Uploading C:\Program Files\Stnexp\Queries\10821663h.str



chain nodes :
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ring nodes :
1 2 3 4 5 16 17 18 19 20
chain bonds :
5-6 6-7 6-15 7-8 7-22 8-9 9-10 9-13 10-11 10-23 11-12 12-14 12-16 20-24 24-25 24-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-5 6-7 6-15 7-8 9-10 9-13 10-11 12-14 12-16 16-17 16-20 24-25 24-26
exact bonds :
2-3 3-4 4-5 5-6 7-22 8-9 10-23 11-12 17-18 18-19 19-20 20-24
isolated ring systems :
containing 1 : 16 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

L33 STRUCTURE UPLOADED

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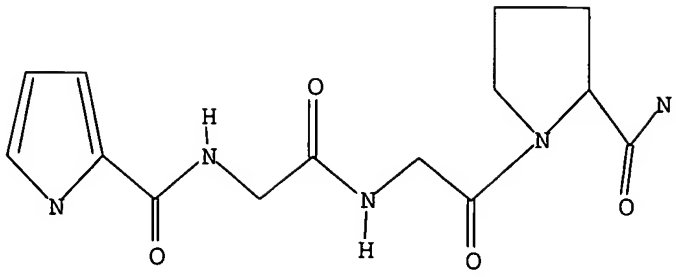
L33 HAS NO ANSWERS
L33 STR



Structure attributes must be viewed using STN Express query preparation.

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100.0% PROCESSED      189 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          2956 TO     4604
PROJECTED ANSWERS:                0 TO        0

L34           0 SEA SSS SAM L33

=> s 133 sss full
FULL SEARCH INITIATED 14:34:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     4154 TO ITERATE

100.0% PROCESSED     4154 ITERATIONS                                7 ANSWERS
SEARCH TIME: 00.00.01

L35           7 SEA SSS FUL L33

=> FIL HCAPLUS
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                  166.94    1592.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00      -7.50

FILE 'HCAPLUS' ENTERED AT 14:34:12 ON 30 NOV 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
```

FILE COVERS 1907 - 30 Nov 2006 VOL 145 ISS 23
FILE LAST UPDATED: 29 Nov 2006 (20061129/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l35
L36 5 L35

=> d his

(FILE 'HOME' ENTERED AT 14:10:49 ON 30 NOV 2006)

FILE 'REGISTRY' ENTERED AT 14:11:13 ON 30 NOV 2006
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L2 50 S L1
L3 28521 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 0 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 0 S L7
L9 0 S L7 SSS FULL
L10 STRUCTURE UPLOADED
L11 0 S L10
L12 0 S L10 SSS FULL
L13 STRUCTURE UPLOADED
L14 50 S L13
L15 28214 S L13 SSS FULL
L16 STRUCTURE UPLOADED
L17 0 S L16
L18 0 S L16 SSS FULL
L19 STRUCTURE UPLOADED
L20 50 S L19
L21 26288 S L19 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:26:01 ON 30 NOV 2006
L22 10499 S L3
L23 35 S L22 AND PROTEASE INHIBITORS
L24 0 S L23 AND HVC
L25 0 S L23 AND NS3
L26 1 S L23 AND HEPATITIS
L27 0 S L23 AND VIRUS IHHIBITOR
L28 9 S L23 AND VIRUS

FILE 'REGISTRY' ENTERED AT 14:32:02 ON 30 NOV 2006
L29 STRUCTURE UPLOADED
L30 0 S L29
L31 1 S L29 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:32:38 ON 30 NOV 2006

L32 3 S L31

FILE 'REGISTRY' ENTERED AT 14:33:42 ON 30 NOV 2006
L33 STRUCTURE UPLOADED
L34 0 S L33
L35 7 S L33 SSS FULL

FILE 'HCAPLUS' ENTERED AT 14:34:12 ON 30 NOV 2006
L36 5 S L35

=> d l32 ibib abs hitstr tot

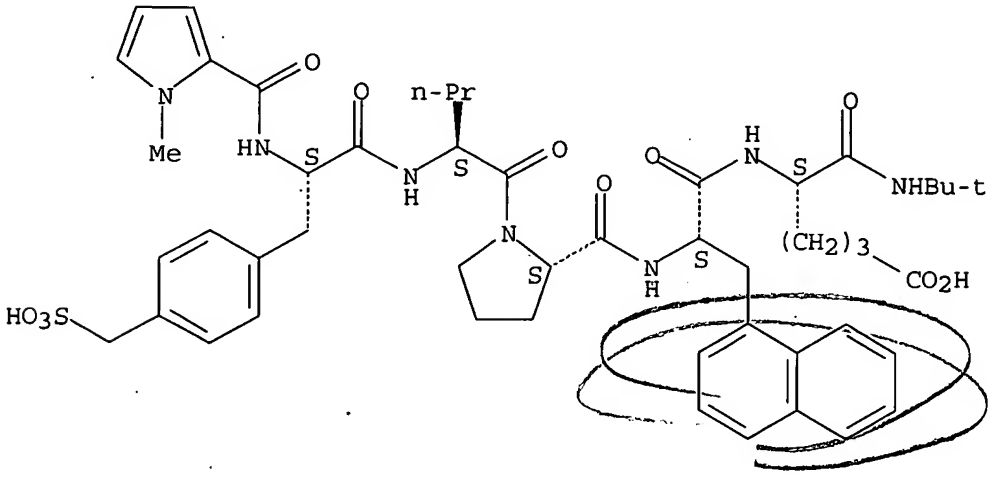
L32 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:928230 HCAPLUS
DOCUMENT NUMBER: 138:19472
TITLE: Method of identifying inhibitors of Cdc25 using three dimensional crystal structure of the catalytic domain of cdc25
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): Australia
SOURCE: U.S. Pat. Appl. Publ., 246 pp., Cont.-in-part of U.S. Ser. No. 645,750.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002183249	A1	20021205	US 2001-797500		20010301
PRIORITY APPLN. INFO.:			US 1999-172215P	P	19990831
			US 2000-645750	A2	20000824

OTHER SOURCE(S): MARPAT 138:19472
AB The present invention relates to the x-ray crystallog. study of proteins comprising the catalytic domains of Cdc25. The atomic coordinates which result from this study are of use in identifying compds. which fit in the catalytic domain and are, therefore, potential inhibitors of Cdc25. The present invention further provides proteins which comprise the ligand binding domain of Cdc25, crystalline forms of these proteins and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Cdc25. The invention also relates to the use of the three dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. These Cdc25 inhibitors are of use in methods of treating a patient having a condition which is modulated by Cdc25 activity, for example, a condition characterized by excessive, inappropriate or undesirable cellular proliferation such as cancer.
IT 329274-31-9P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of identifying inhibitors of Cdc25 using three dimensional

crystal structure of catalytic domain of Cdc25)
RN 329274-31-9 HCAPLUS
CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L32 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:696111 HCAPLUS
DOCUMENT NUMBER: 137:228607
TITLE: Crystal structure and three-dimensional structure of human Cdc25 catalytic domains and its use in designing peptidomimetic inhibitors
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany; GPC Biotech Inc.
SOURCE: PCT Int. Appl., 351 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002070680	A1	20020912	WO 2001-US6587	20010301
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			WO 2001-US6587	20010301

OTHER SOURCE(S): MARPAT 137:228607

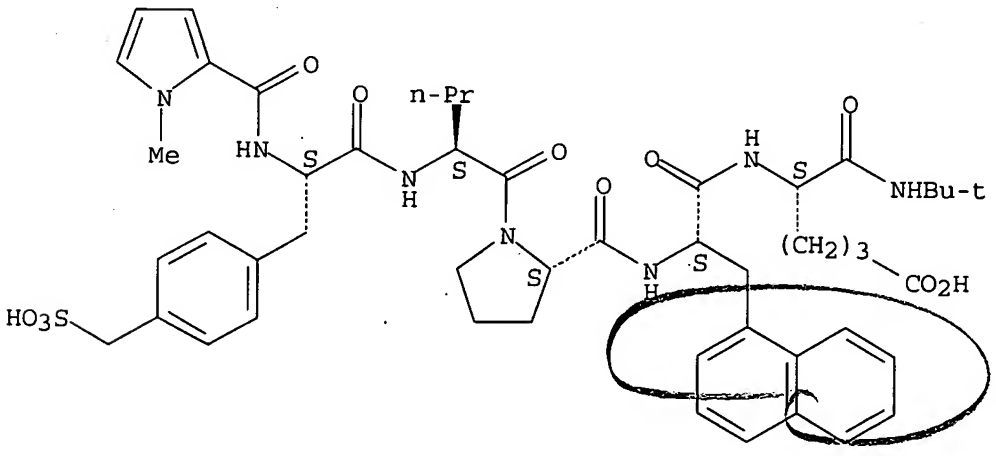
AB Due to its role in regulating the cell cycle, Cdc25 (a family of dual specificity phosphatases) is a potential target for therapies aimed at controlling proliferative diseases, but rational, structure-based design has not been possible because of the lack of accurate 3-dimensional data. The present invention relates to polypeptides which comprises the ligand binding domain of human Cdc25 proteins, crystalline forms of these polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of Cdc25. In particular, a high resolution crystal structure was obtained for the polypeptide denoted CDC25B(ΔN8B), comprising residues Glu-368 through Arg-562 of human Cdc25B, complexed with a pentapeptide inhibitor denoted cdc1249 (2-methoxynaphthyl-1-carboxy-(4-sulfomethyl)-L-Phe-L-Glu-L-Glu-L-naphthylalanine-L-Glu-amide). The invention also relates to the use of the 3-dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. The syntheses and structures of a large number of putative pentapeptide inhibitors are also provided. Such inhibitors have potential in the treatment of diseases associated with excessive cellular proliferation, such as cancer, restenosis, reocclusion of coronary artery, and inflammation.

IT 329274-31-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(crystal structure and three-dimensional structure of human Cdc25 catalytic domains and its use in designing peptidomimetic inhibitors)

RN 329274-31-9 HCAPLUS

CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:168124 HCAPLUS
DOCUMENT NUMBER: 134:218936
TITLE: Crystal structure of CDC25 proteins and its use in

rational design of inhibitors

INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016300	A2	20010308	WO 2000-US23473	20000825
WO 2001016300	A3	20020530		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2383603	AA	20010308	CA 2000-2383603	20000825
EP 1226237	A2	20020731	EP 2000-959449	20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: US 1999-172215P P 19990831
WO 2000-US23473 W 20000825

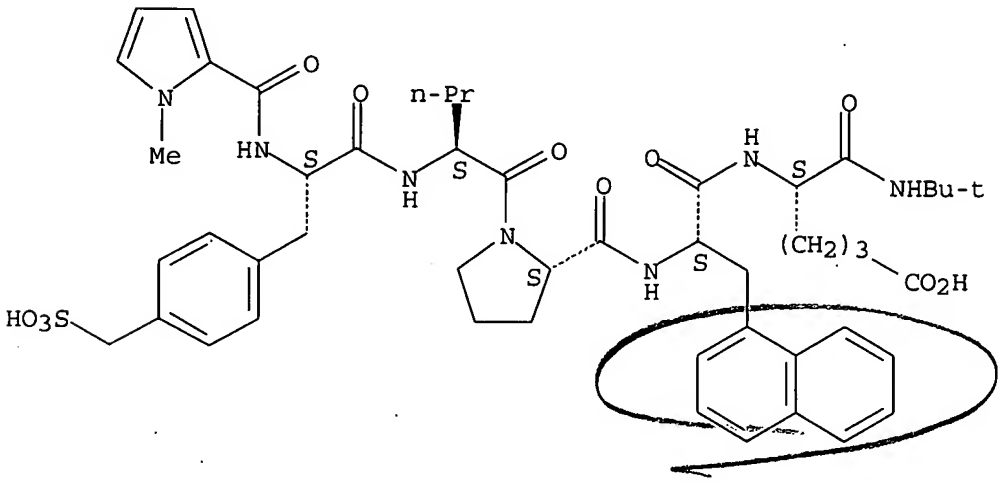
OTHER SOURCE(S): MARPAT 134:218936

AB The present invention relates to polypeptides which comprise the ligand binding domain of CDC25, crystalline forms of these polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of CDC25 alone and in complexes with pentapeptide inhibitors. Atomic coordinates are provided from x-ray diffraction of crystals of CDC25A and CDC25B catalytic domains in the presence and absence of various inhibitors. The invention also relates to the use of the 3-dimensional structure of the CDC25 catalytic domain in methods of designing and/or identifying potential inhibitors of CDC25 activity, for example, compds. which inhibit the binding of a native substrate to the CDC25 catalytic domain. The method comprises the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the CDC25 catalytic domain, and (2) identifying a scaffold which presents the functional group or functional groups in a suitable orientation for interacting with one or more subsites of the CDC25 catalytic domain. Since CDC25 is a potential target for therapies aimed at controlling proliferative disease, the atomic coordinates allow rational structure-based design of potential agents for the treatment of cancer, restenosis, reocclusion of coronary artery, or inflammation.

IT 329274-31-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure of CDC25 proteins and its use in rational design of

inhibitors)
RN 329274-31-9 HCAPLUS
CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI). (CA INDEX NAME)

Absolute stereochemistry.



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L36 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:902372 HCAPLUS
DOCUMENT NUMBER: 141:350404
TITLE: Preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease
INVENTOR(S): Farmer, Luc J.; Perni, Robert P.; Bhisetti, Govinda Rao; Wilson, Keith P.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Incorporated, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092162	A1	20041028	WO 2004-US11012	20040409
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004018986	A1	20040129	US 2003-412600	20030411

AU 2004230946	A1	20041028	AU 2004-230946	20040409
CA 2521678	AA	20041028	CA 2004-2521678	20040409
US 2005090450	A1	20050428	US 2004-821793	20040409
EP 1636208	A1	20060322	EP 2004-759362	20040409
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CN 1795188	A	20060628	CN 2004-80014047	20040409
JP 2006526011	T2	20061116	JP 2006-509873	20040409

PRIORITY APPLN. INFO.:

US 2003-412600	A	20030411
US 2003-513765P	P	20031023
US 2002-371846P	P	20020411
WO 2004-US11012	W	20040409

OTHER SOURCE(S): MARPAT 141:350404

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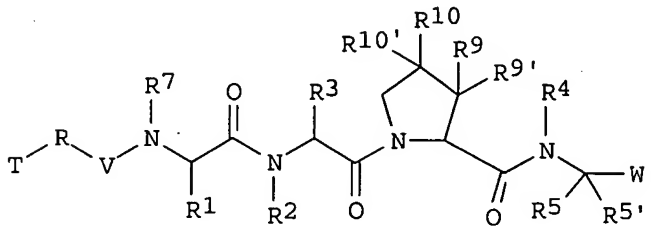

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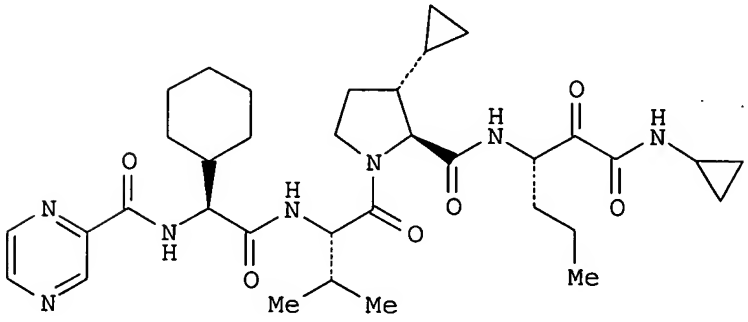


II

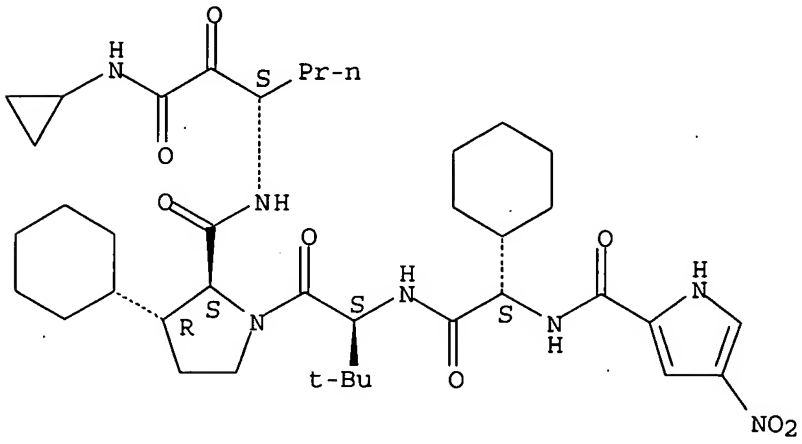
AB The invention relates to compds. I [the R groups are H (except R1, R3) or various groups, i.e., R5, R5' are alkyl, halo-, mercapto- or hydroxyalkyl, (un)substituted Ph or benzyl or R5/R5' may form a ring; R2, R4, R7 are (un)substituted alkyl, cycloalkylalkyl or arylalkyl; R1, R3 are (un)substituted alkyl, cycloalkyl, cycloalkylalkyl, etc.; R9, R9', R10, R10' are -X-Y-Z, where X is a bond, alkylene, O, S or imino, Y is a bond, CH2, CO, COCO, SO, SO2 or sulfinylimino, Z is H, alkyl, aryl, etc.; V is CO, SO or SO2, R is CO, SO, SO2, imino, O or a bond; T is alkyl, aryl, etc; W is an acyl or boryl group] or their pharmaceutically-acceptable salts that inhibit serine protease activity, particularly the activity of hepatitis C virus (HCV) NS3-NS4A protease. Thus, peptide II was prepared by peptide coupling reactions in solution and showed Ki in the range 0.5-1 μM for inhibition of HCV.

IT 777087-40-8P 777087-41-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease)

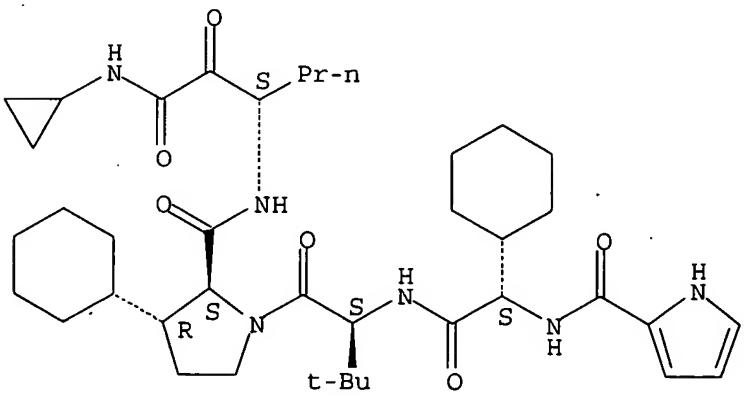
RN 777087-40-8 HCAPLUS
CN L-Prolinamide, 4-nitro-1H-pyrrole-2-carbonyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-3-cyclohexyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 777087-41-9 HCAPLUS
CN L-Prolinamide, 1H-pyrrole-2-carbonyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-3-cyclohexyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



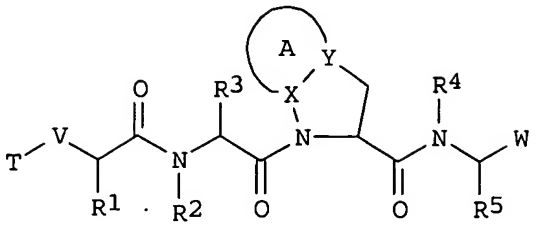
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:837079 HCAPLUS
DOCUMENT NUMBER: 139:338195
TITLE: Preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease

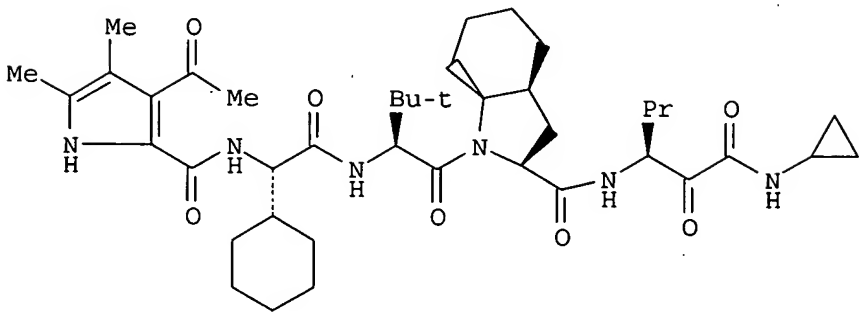
INVENTOR(S): Pitlik, Janos; Cottrell, Kevin M.; Farmer, Luc J.; Perni, Robert B.; Courtney, Lawrence F.; Van Drie, John H.; Murcko, Mark A.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 210 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003087092	A2	20031023	WO 2003-US11459	20030411
WO 2003087092	A3	20040910		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2481369	AA	20031023	CA 2003-2481369	20030411
AU 2003223602	A1	20031027	AU 2003-223602	20030411
EP 1497282	A2	20050119	EP 2003-719741	20030411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1649864	A	20050803	CN 2003-809665	20030411
JP 2005535574	T2	20051124	JP 2003-584048	20030411
NO 2004004889	A	20050110	NO 2004-4889	20041110
PRIORITY APPLN. INFO.:			US 2002-371846P P	20020411
			WO 2003-US11459 W	20030411

OTHER SOURCE(S): MARPAT 139:338195
GI



I



II

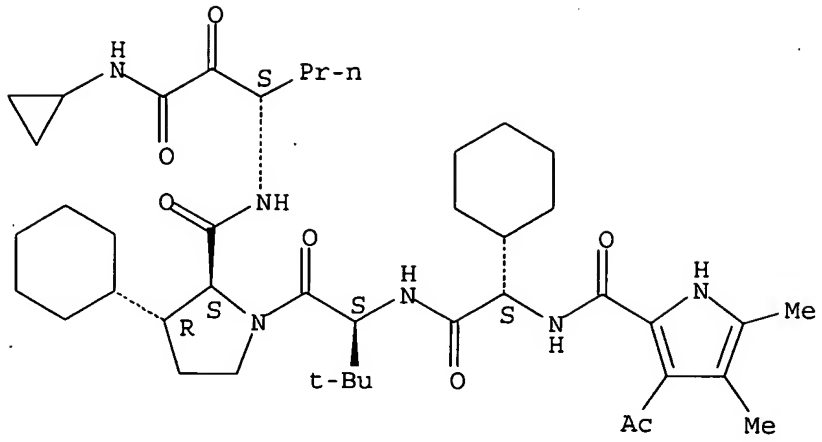
AB The invention relates to compds. I [A together with X and Y is a 3- to 6-membered aromatic or non-aromatic ring having up to 3 heteroatoms; R1, R3 are aliphatic, (un)substituted (cyclo)alk(en)yl, (hetero)aryl, etc.; R2, R4 are H, (un)substituted aliphatic, cycloalkyl or aryl aliphatic; R5 is (un)substituted aliphatic; W is COCOR6, COCO2R6, or COCONR62, where R6 is H, aliphatic, (hetero)aryl, etc.; V is CONR8, SONR8, SO2NR8, where R8 is H or aliphatic; T is (hetero)aryl, aliphatic, sulfonylaminoalkyl, etc.] that inhibit serine protease activity, particularly the activity of hepatitis C virus NS3-NS4A protease. Thus, peptide II was prepared via coupling reactions in solution and showed Ki and IC50 values < 0.5 μM.

IT 615584-02-6P 615584-03-7P 615584-04-8P
615584-05-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of serine proteases, particularly HCV NS3-NS4A protease)

RN 615584-02-6 HCAPLUS

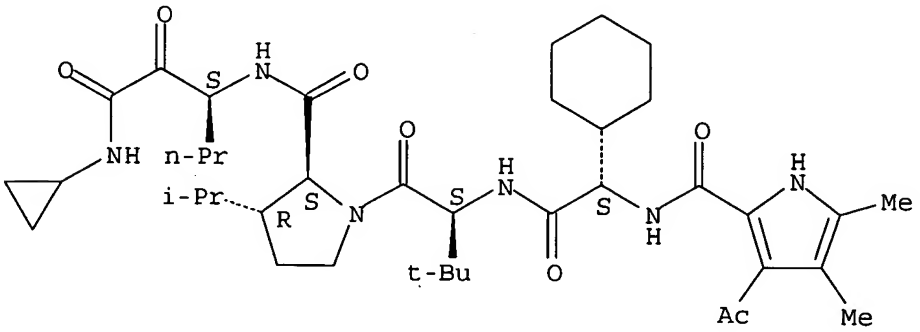
CN L-Prolinamide, 3-acetyl-2,3,4,5-tetradehydro-4,5-dimethylprolyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-3-cyclohexyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



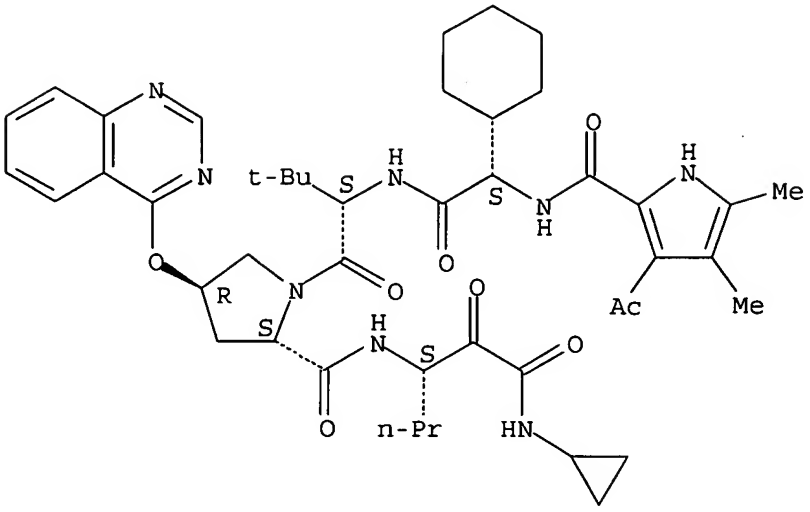
RN 615584-03-7 HCAPLUS
CN L-Prolinamide, 3-acetyl-2,3,4,5-tetradehydro-4,5-dimethylprolyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-3-(1-methylethyl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



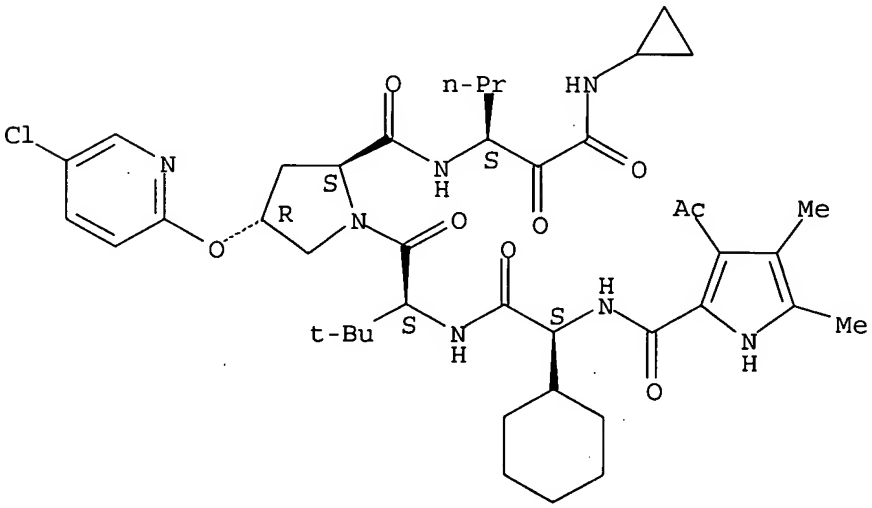
RN 615584-04-8 HCAPLUS
CN L-Prolinamide, 3-acetyl-2,3,4,5-tetradehydro-4,5-dimethylprolyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-4-(4-quinazolinyloxy)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 615584-05-9 HCAPLUS
CN L-Prolinamide, 3-acetyl-2,3,4,5-tetradehydro-4,5-dimethylprolyl-(2S)-2-cyclohexylglycyl-3-methyl-L-valyl-4-[(5-chloro-2-pyridinyl)oxy]-N-[(1S)-1-[(cyclopropylamino)oxoacetyl]butyl]-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:928230 HCAPLUS
DOCUMENT NUMBER: 138:19472
TITLE: Method of identifying inhibitors of Cdc25 using three dimensional crystal structure of the catalytic domain of Cdc25
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah;

Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): Australia
SOURCE: U.S. Pat. Appl. Publ., 246 pp., Cont.-in-part of U.S. Ser. No. 645,750.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2002183249	A1	20021205	US 2001-797500		20010301
PRIORITY APPLN. INFO.:			US 1999-172215P	P	19990831
			US 2000-645750	A2	20000824

OTHER SOURCE(S): MARPAT 138:19472

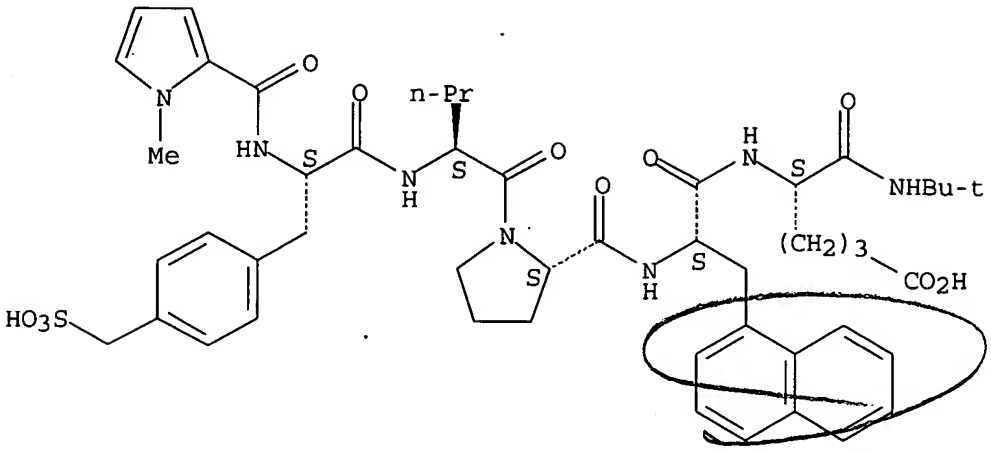
AB The present invention relates to the x-ray crystallog. study of proteins comprising the catalytic domains of Cdc25. The atomic coordinates which result from this study are of use in identifying compds. which fit in the catalytic domain and are, therefore, potential inhibitors of Cdc25. The present invention further provides proteins which comprise the ligand binding domain of Cdc25, crystalline forms of these proteins and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Cdc25. The invention also relates to the use of the three dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. These Cdc25 inhibitors are of use in methods of treating a patient having a condition which is modulated by Cdc25 activity, for example, a condition characterized by excessive, inappropriate or undesirable cellular proliferation such as cancer.

IT 329274-31-9P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of identifying inhibitors of Cdc25 using three dimensional crystal structure of catalytic domain of Cdc25)

RN 329274-31-9 HCAPLUS

CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L36 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:696111 HCAPLUS
DOCUMENT NUMBER: 137:228607
TITLE: Crystal structure and three-dimensional structure of human Cdc25 catalytic domains and its use in designing peptidomimetic inhibitors
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark
PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany; GPC Biotech Inc.
SOURCE: PCT Int. Appl., 351 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002070680	A1	20020912	WO 2001-US6587	20010301

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: WO 2001-US6587 20010301
OTHER SOURCE(S): MARPAT 137:228607

AB Due to its role in regulating the cell cycle, Cdc25 (a family of dual specificity phosphatases) is a potential target for therapies aimed at controlling proliferative diseases, but rational, structure-based design has not been possible because of the lack of accurate 3-dimensional data. The present invention relates to polypeptides which comprises the ligand binding domain of human Cdc25 proteins, crystalline forms of these

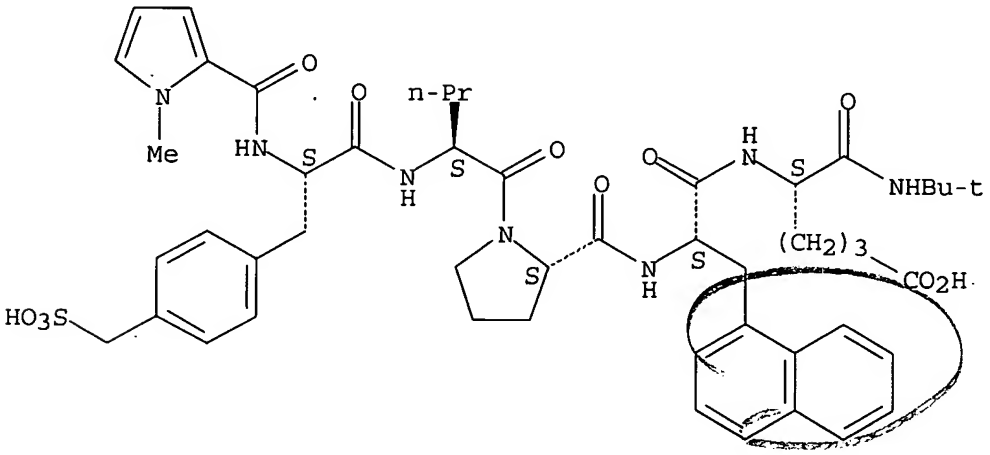
polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of Cdc25. In particular, a high resolution crystal structure was obtained for the polypeptide denoted CDC25B(ΔN8B), comprising residues Glu-368 through Arg-562 of human Cdc25B, complexed with a pentapeptide inhibitor denoted cdc1249 (2-methoxynaphthyl-1-carboxy-(4-sulfomethyl)-L-Phe-L-Glu-L-Glu-L-naphthylalanine-L-Glu-amide). The invention also relates to the use of the 3-dimensional structure of the Cdc25 catalytic domain in methods of designing and/or identifying potential inhibitors of Cdc25 activity, for example, compds. which inhibitors of Cdc25 activity, for example, compds. which inhibit the binding of a native substrate to the Cdc25 catalytic domain. The syntheses and structures of a large number of putative pentapeptide inhibitors are also provided. Such inhibitors have potential in the treatment of diseases associated with excessive cellular proliferation, such as cancer, restenosis, reocclusion of coronary artery, and inflammation.

IT 329274-31-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(crystal structure and three-dimensional structure of human Cdc25 catalytic domains and its use in designing peptidomimetic inhibitors)

RN 329274-31-9 HCAPLUS

CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:168124 HCAPLUS
DOCUMENT NUMBER: 134:218936
TITLE: Crystal structure of CDC25 proteins and its use in rational design of inhibitors
INVENTOR(S): Taylor, Neil R.; Borhani, David; Epstein, David; Rudolph, Johannes; Ritter, Kurt; Fujimori, Taro; Robinson, Simon; Eckstein, Jens; Haupt, Andreas; Walker, Nigel; Dixon, Richard W.; Choquette, Deborah; Blanchard, Jill; Kluge, Arthur; Pal, Kollol; Bockovich, Nicholas; Come, Jon; Hediger, Mark

PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 314 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001016300	A2	20010308	WO 2000-US23473	20000825
WO 2001016300	A3	20020530		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2383603	AA	20010308	CA 2000-2383603	20000825
EP 1226237	A2	20020731	EP 2000-959449	20000825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: US 1999-172215P P 19990831
WO 2000-US23473 W 20000825

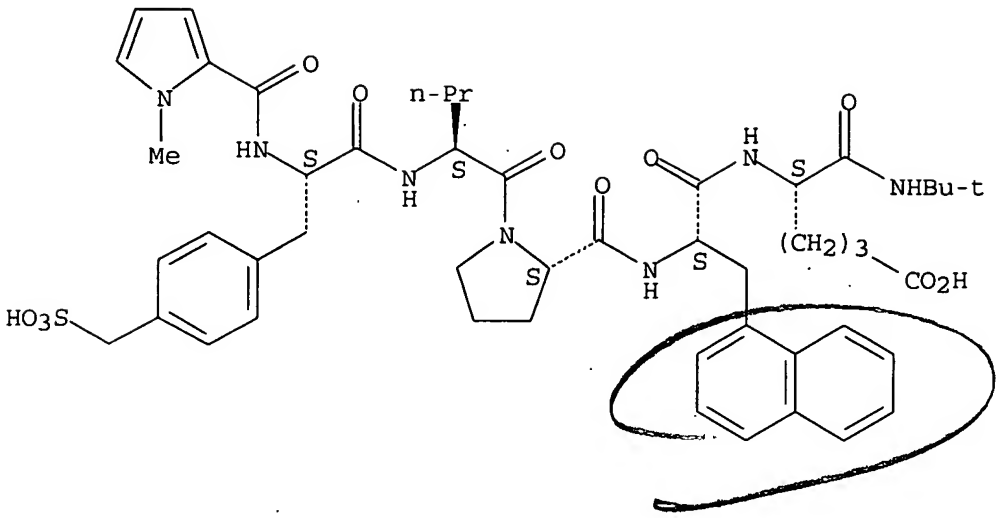
OTHER SOURCE(S): MARPAT 134:218936

AB The present invention relates to polypeptides which comprise the ligand binding domain of CDC25, crystalline forms of these polypeptides, and the use of these crystalline forms to determine the 3-dimensional structure of the catalytic domain of CDC25 alone and in complexes with pentapeptide inhibitors. Atomic coordinates are provided from x-ray diffraction of crystals of CDC25A and CDC25B catalytic domains in the presence and absence of various inhibitors. The invention also relates to the use of the 3-dimensional structure of the CDC25 catalytic domain in methods of designing and/or identifying potential inhibitors of CDC25 activity, for example, compds. which inhibit the binding of a native substrate to the CDC25 catalytic domain. The method comprises the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the CDC25 catalytic domain, and (2) identifying a scaffold which presents the functional group or functional groups in a suitable orientation for interacting with one or more subsites of the CDC25 catalytic domain. Since CDC25 is a potential target for therapies aimed at controlling proliferative disease, the atomic coordinates allow rational structure-based design of potential agents for the treatment of cancer, restenosis, reocclusion of coronary artery, or inflammation.

IT 329274-31-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystal structure of CDC25 proteins and its use in rational design of inhibitors)

RN 329274-31-9 HCAPLUS
CN L-Norvalinamide, 2,3,4,5-tetradehydro-1-methylprolyl-4-(sulfomethyl)-L-phenylalanyl-L-norvalyl-L-prolyl-3-(1-naphthalenyl)-L-alanyl-5-carboxy-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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FULL ESTIMATED COST	58.59	1650.64
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.00	-13.50

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